

chain nodes :

10

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

1-10

ring bonds :

1-2 1-7 2-3 3-4 3-5 4-8 5-6 6-9 7-8 8-9

exact/norm bonds :

1-2 1-7 1-10 2-3 3-4 3-5 4-8 5-6 6-9 7-8 8-9

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom

Welcome to STN International! Enter x:x

LOGINID:sssptal611hxl

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4 Apr 09 ZDB will be removed from STN
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and
IFIUDB
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and
ZCAPLUS
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available
NEWS 9 Jun 03 New e-mail delivery for search results now available
NEWS 10 Jun 10 MEDLINE Reload
NEWS 11 Jun 10 PCTFULL has been reloaded
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
saved answer sets no longer valid
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY
NEWS 15 Jul 30 NETFIRST to be removed from STN
NEWS 16 Aug 08 CANCERLIT reload
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18 Aug 08 NTIS has been reloaded and enhanced
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
now available on STN
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file
NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:35:52 ON 22 SEP 2002

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 11:36:00 ON 22 SEP 2002

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 SEP 2002 HIGHEST RN 453593-49-2

DICTIONARY FILE UPDATES: 20 SEP 2002 HIGHEST RN 453593-49-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>

Uploading C:\STNEXP4\QUERIES\09864905.str

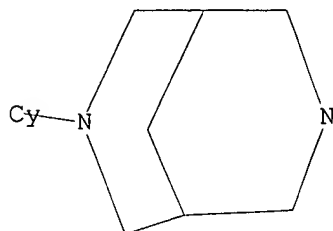
L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

Hong Liu

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 11:36:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9550 TO ITERATE

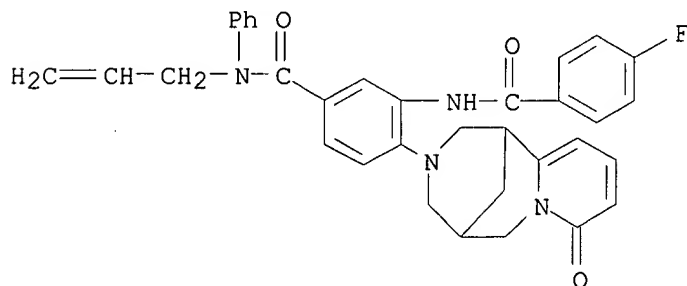
10.5% PROCESSED 1000 ITERATIONS 6 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 185150 TO 196850
PROJECTED ANSWERS: 692 TO 1600

L3 6 SEA SSS SAM L1

=> d scan

L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzamide, 3-[(4-fluorobenzoyl)amino]-N-phenyl-N-2-propenyl-4-(1,5,6,8-tetrahydro-8-oxo-1,5-methano-2H-pyrido[1,2-a][1,5]diazocin-3(4H)-yl)-(9CI)
MF C34 H31 F N4 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Hong Liu

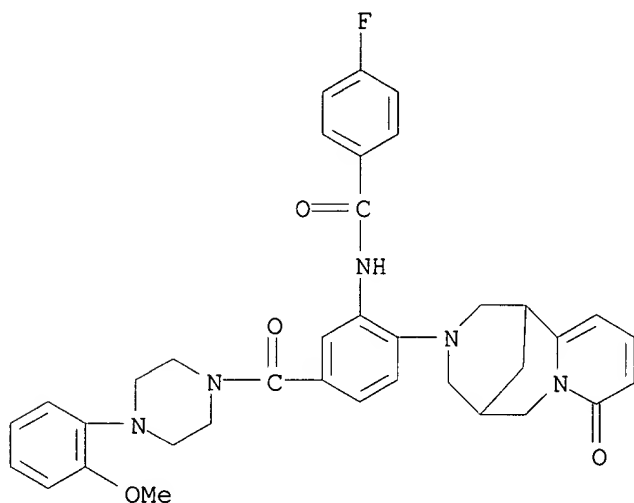
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide, 4-fluoro-N-[5-[[4-(2-methoxyphenyl)-1-piperazinyl]carbonyl]-2-

(1,5,6,8-tetrahydro-8-oxo-1,5-methano-2H-pyrido[1,2-a][1,5]diazocin-3(4H)-yl)phenyl]- (9CI)

MF C36 H36 F N5 O4



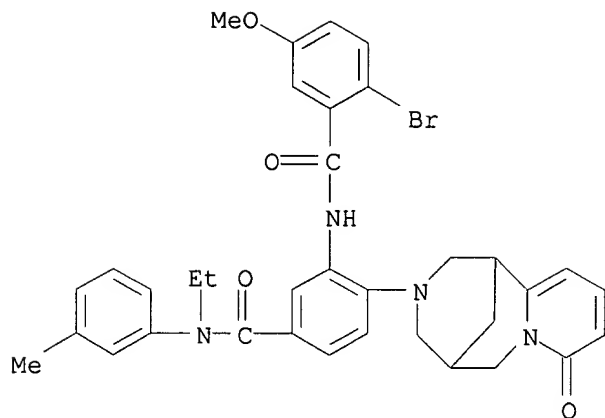
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzamide,

3-[(2-bromo-5-methoxybenzoyl)amino]-N-ethyl-N-(3-methylphenyl)-4-(1,5,6,8-tetrahydro-8-oxo-1,5-methano-2H-pyrido[1,2-a][1,5]diazocin-3(4H)-yl)- (9CI)

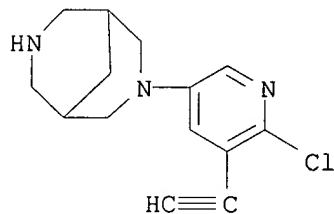
MF C35 H35 Br N4 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

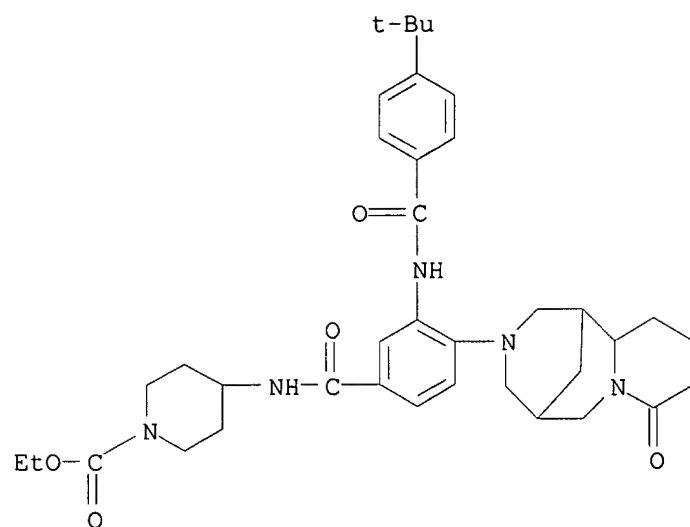
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-5-ethynyl-3-pyridinyl)- (9CI)
 MF C14 H16 Cl N3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 6 ANSWERS REGISTRY COPYRIGHT 2002 ACS
 IN 1-Piperidinecarboxylic acid,
 4-[[3-[[4-(1,1-dimethylethyl)benzoyl]amino]-4-(
 (octahydro-8-oxo-1,5-methano-2H-pyrido[1,2-a][1,5]diazocin-3(4H)-
 yl)benzoyl]amino]-, ethyl ester (9CI)
 MF C37 H49 N5 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>

Uploading C:\STNEXP4\QUERIES\09864905.str

L4 STRUCTURE UPLOADED

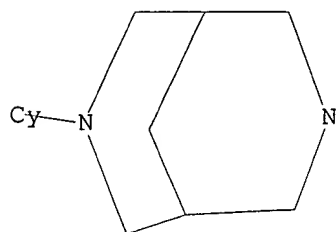
=> que L4

L5 QUE L4

=> d 14

L4 HAS NO ANSWERS

L4 STR



Hong Liu

Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 11:38:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 283 TO ITERATE

100.0% PROCESSED 283 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 4651 TO 6669
PROJECTED ANSWERS: 5 TO 234

L6 5 SEA SSS SAM L4

=> s 16 ful

FULL SEARCH INITIATED 11:39:02 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5707 TO ITERATE

100.0% PROCESSED 5707 ITERATIONS 100 ANSWERS
SEARCH TIME: 00.00.01

L7 100 SEA SSS FUL L4

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	141.80	142.01

FILE 'CAPLUS' ENTERED AT 11:39:10 ON 22 SEP 2002
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FILE COVERS 1907 - 22 Sep 2002 VOL 137 ISS 13
FILE LAST UPDATED: 20 Sep 2002 (20020920/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

Hong Liu

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 17

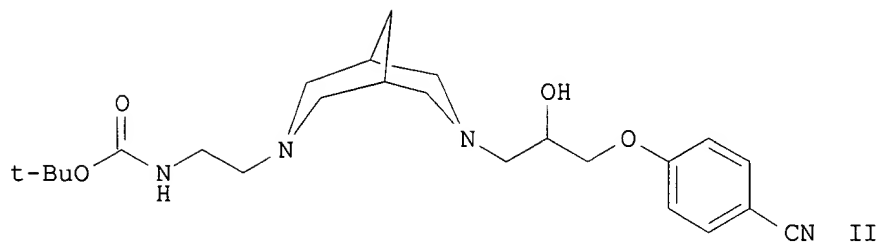
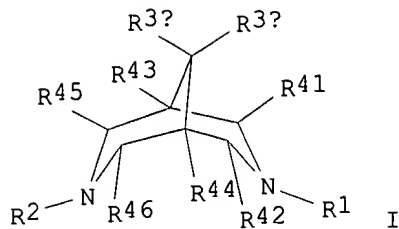
L8 28 L7

=> d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 28 ANSWERS - CONTINUE? Y/(N):y

~~28~~ ANSWER 1 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2002:51458 CAPLUS
 DOCUMENT NUMBER: 136:118479
 TITLE: Preparation of new bispidine compounds for the treatment of cardiac arrhythmias
 INVENTOR(S): Andersson, Kjell; Bjoere, Annika; Bjoersne, Magnus; Ponten, Fritiof; Strandlund, Gert; Svensson, Peder; Tottie, Louise
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
 SOURCE: PCT Int. Appl., 110 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004446	A1	20020117	WO 2001-SE1544	20010704
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001071161	A5	20020121	AU 2001-71161	20010704
PRIORITY APPLN. INFO.:				
			SE 2000-2603	A 20000707
			SE 2000-2788	A 20000727
			WO 2001-SE1544	W 20010704
OTHER SOURCE(S): MARPAT 136:118479				
GI				



AB The title compds. [I; R1 = ACR4R5BR6 (wherein R4 = H, halo, alkyl, etc.; or R4, together with R5, = O; R5 = H, alkyl,; A = a bond, alkylene, etc.; B = a bond, alkylene, etc.; R6 = (un)substituted aryl, 5-12 membered heterocyclyl contg. one or more heteroatoms selected from O, N and/or S); R2 = CN, (un)substituted 5-12 membered heterocyclyl contg. one or more heteroatoms selected from O, N and/or S, etc.; R3a, R3b = H, alkyl, etc.; or R3a and R3b together = alkylene, O(alkylene)O, etc.; R41-R46 = H, alkyl] which are useful in the prophylaxis and in the treatment of arrhythmias, in particular atrial and ventricular arrhythmias, were prepd.

E.g., a 3-step synthesis of II was given. The exemplified compds. I showed pIC50 of at least 5.5 in glucocorticoid-treated mouse fibroblasts as a model to detect blockers of the delayed rectifier K current.

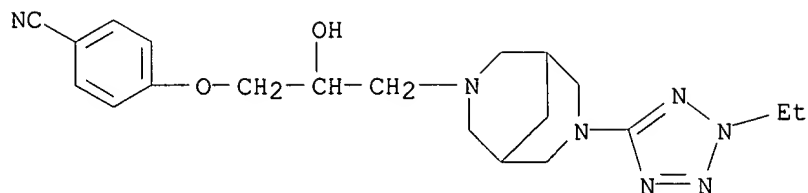
IT 389885-68-1P 389885-69-2P 389886-19-5P
 389886-27-5P 389886-28-6P 389886-29-7P
 389886-44-6P 389886-54-8P 389886-70-8P
 389886-88-8P 389886-89-9P 389886-90-2P
 389886-91-3P 389887-29-0P 389887-30-3P
 389887-66-5P 389887-67-6P 389887-68-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of new bispidine compds. for the treatment of cardiac arrhythmias)

RN 389885-68-1 CAPLUS

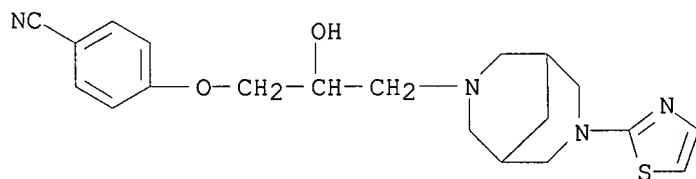
CN Benzonitrile, 4-[3-[7-(2-ethyl-2H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)



RN 389885-69-2 CAPLUS

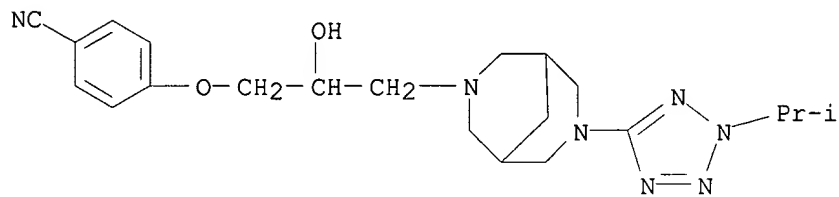
CN Benzonitrile,

4-[2-hydroxy-3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



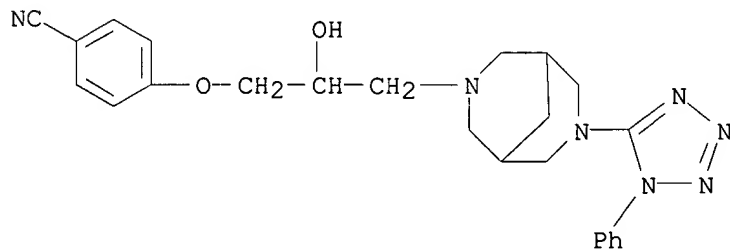
RN 389886-19-5 CAPLUS

CN Benzonitrile, 4-[2-hydroxy-3-[7-[2-(1-methylethyl)-2H-tetrazol-5-yl]-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



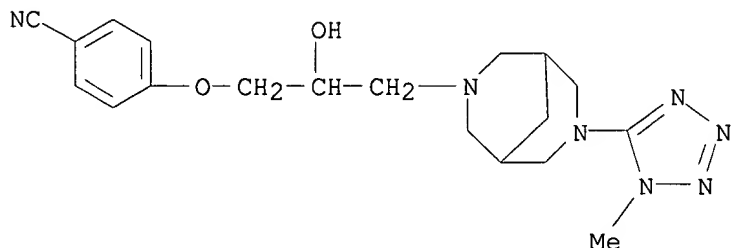
RN 389886-27-5 CAPLUS

CN Benzonitrile, 4-[2-hydroxy-3-[7-(1-phenyl-1H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



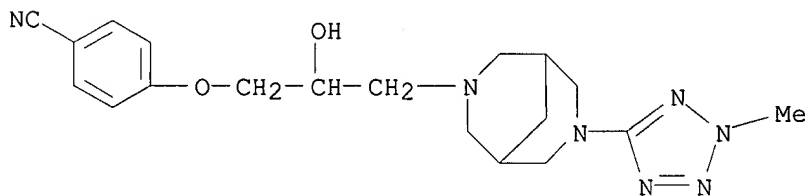
RN 389886-28-6 CAPLUS

CN Benzonitrile, 4-[2-hydroxy-3-[7-(1-methyl-1H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



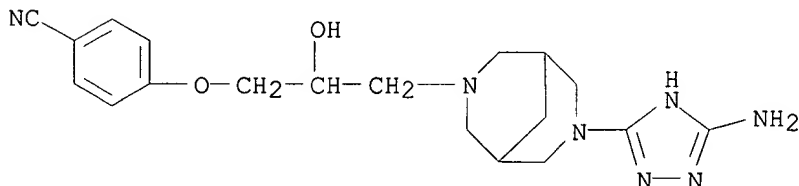
RN 389886-29-7 CAPLUS

CN Benzonitrile, 4-[2-hydroxy-3-[7-(2-methyl-2H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



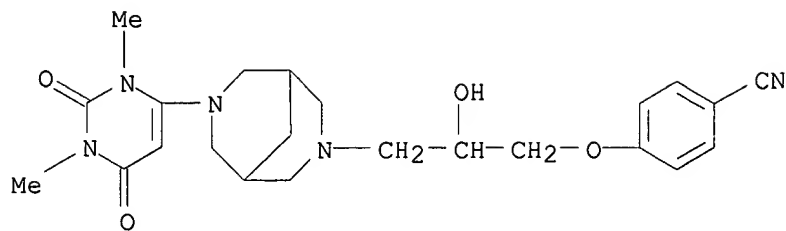
RN 389886-44-6 CAPLUS

CN Benzonitrile, 4-[3-[7-(5-amino-1H-1,2,4-triazol-3-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)



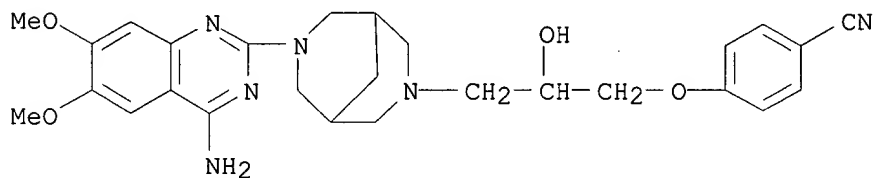
RN 389886-54-8 CAPLUS

CN Benzonitrile, 4-[2-hydroxy-3-[7-(1,2,3,6-tetrahydro-1,3-dimethyl-2,6-dioxo-4-pyrimidinyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]- (9CI) (CA INDEX NAME)



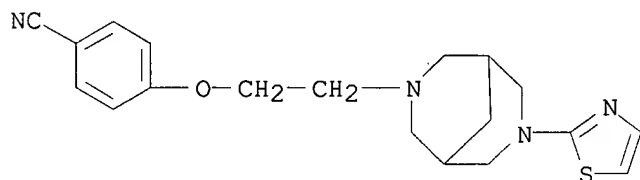
RN 389886-70-8 CAPLUS

CN Benzonitrile, 4-[3-[7-(4-amino-6,7-dimethoxy-2-quinazolinyl)-3,7-diazabicyclo[3.3.1]non-3-yl]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)



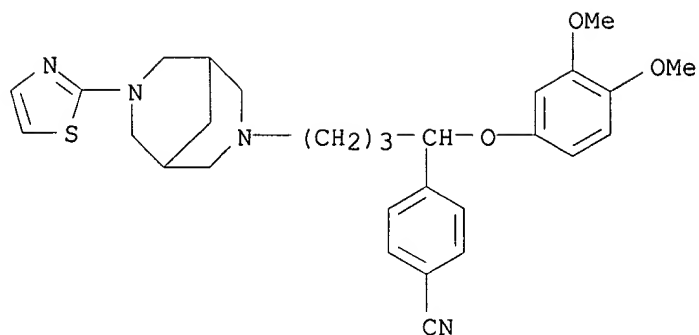
RN 389886-88-8 CAPLUS

CN Benzonitrile, 4-[2-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]ethoxy]- (9CI) (CA INDEX NAME)



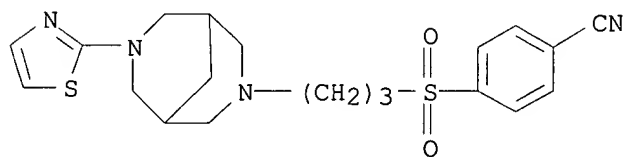
RN 389886-89-9 CAPLUS

CN Benzonitrile, 4-[1-(3,4-dimethoxyphenoxy)-4-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]butyl]- (9CI) (CA INDEX NAME)



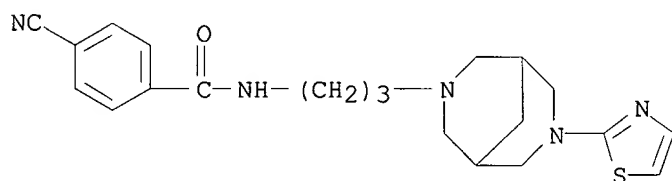
RN 389886-90-2 CAPLUS

CN Benzonitrile, 4-[[3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propyl]sulfonyl]- (9CI) (CA INDEX NAME)



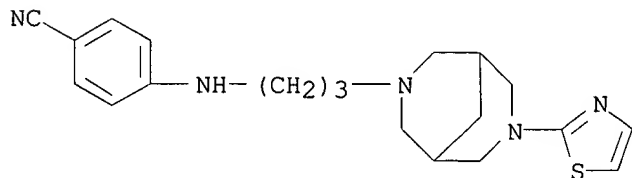
RN 389886-91-3 CAPLUS

CN Benamide, 4-cyano-N-[3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propyl]- (9CI) (CA INDEX NAME)

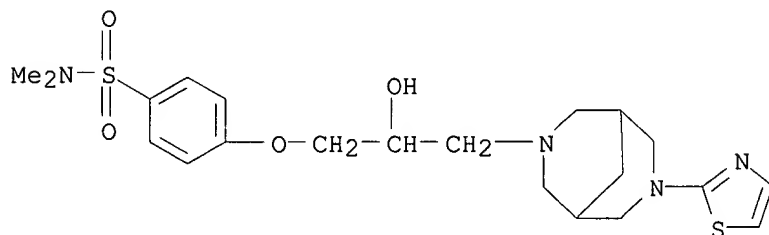


RN 389887-29-0 CAPLUS

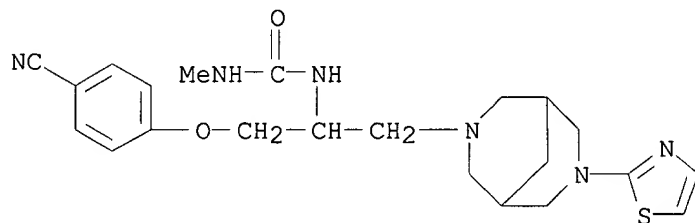
CN Benzonitrile, 4-[[3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propyl]amino]- (9CI) (CA INDEX NAME)



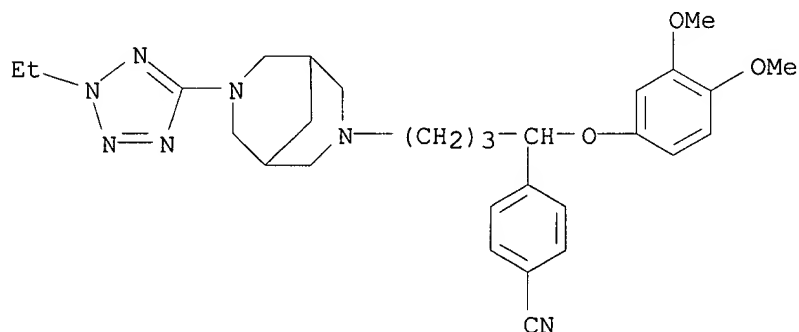
RN 389887-30-3 CAPLUS
 CN Benzenesulfonamide, 4-[2-hydroxy-3-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]propoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



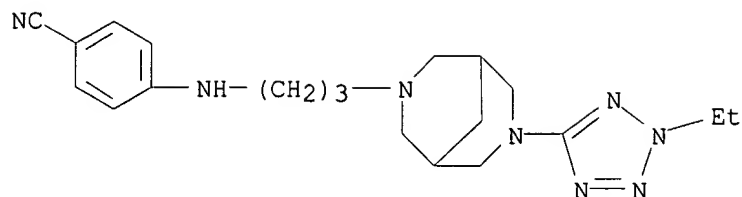
RN 389887-66-5 CAPLUS
 CN Urea, N-[1-[(4-cyanophenoxy)methyl]-2-[7-(2-thiazolyl)-3,7-diazabicyclo[3.3.1]non-3-yl]ethyl]-N'-methyl- (9CI) (CA INDEX NAME)



RN 389887-67-6 CAPLUS
 CN Benzonitrile,
 4-[1-(3,4-dimethoxyphenoxy)-4-[7-(2-ethyl-2H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]butyl]- (9CI) (CA INDEX NAME)



RN 389887-68-7 CAPLUS
 CN Benzonitrile, 4-[[3-[7-(2-ethyl-2H-tetrazol-5-yl)-3,7-diazabicyclo[3.3.1]non-3-yl]propyl]amino]- (9CI) (CA INDEX NAME)

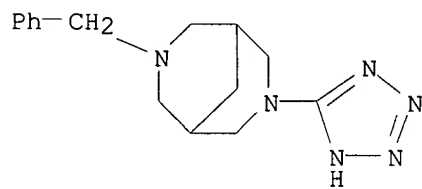


IT **389887-70-1P 389887-71-2P 389887-72-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of new bispidine compds. for the treatment of cardiac arrhythmias)

RN 389887-70-1 CAPLUS

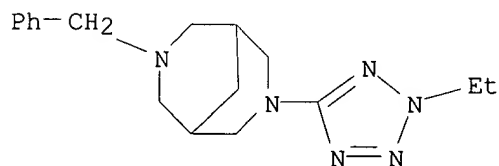
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)-7-(1H-tetrazol-5-yl)-, ammonium salt (9CI) (CA INDEX NAME)



● NH₃

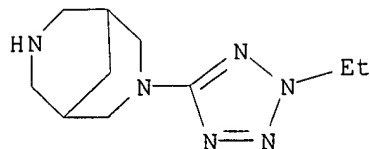
RN 389887-71-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-ethyl-2H-tetrazol-5-yl)-7-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 389887-72-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-ethyl-2H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 2 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:453062 CAPLUS

DOCUMENT NUMBER: 135:61360

TITLE: Preparation of heteroaryldiazabicycloalkanes as nicotinic cholinergic receptor ligands.

INVENTOR(S): Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Nielsen, Simon Feldbaek; Ahning, Philip K.; Jorgensen, Tino Dyhring

PATENT ASSIGNEE(S): Neurosearch A/S, Den.

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

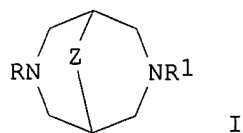
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001044243	A2	20010621	WO 2000-DK696	20001214
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			DK 1999-1790	A 19991214
OTHER SOURCE(S):			MARPAT 135:61360	
GI				



AB Title compds. [I; Z = (CH₂)_n; n = 0-2; R = H, alkyl, aryl, aralkyl,

Hong Liu

fluorescent group; R1 = (substituted) mono- or polyheterocyclyl], were prepd. as drugs and diagnostic agents (no data). Thus, 3,7-dibenzyl-3,7-diazabicyclo[3.3.1]nonane (prepn. given) was stirred with

HCO₂H and Pd/C to give crude monobenzyl deriv., which was heated with 2-chloroquinoline at 100.degree. for 1 h to give 7-benzyl-3-(2-quinolinyl)-

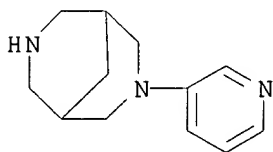
3,7-diazabicyclo[3.3.1]nonane. I may be useful for the treatment of central nervous system diseases, disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neurodegeneration inflammation, pain, and drug withdrawal symptoms.

IT 286945-99-1P 286946-00-7P 286946-07-4P
345317-15-9P 345317-16-0P 345317-17-1P
345317-18-2P 345317-19-3P 345317-20-6P
345317-21-7P 345317-22-8P 345317-23-9P
345317-24-0P 345317-25-1P 345317-26-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of heteroaryldiazabicycloalkanes as nicotinic cholinergic receptor ligands)

RN 286945-99-1 CAPLUS

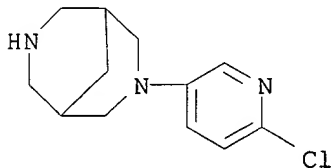
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(3-pyridinyl)- (9CI) (CA INDEX NAME)



546/122
514/300

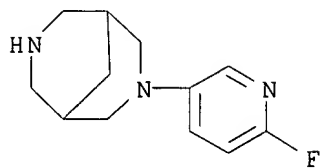
RN 286946-00-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)

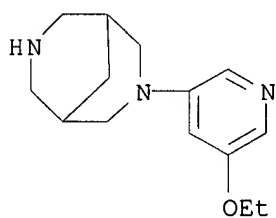


RN 286946-07-4 CAPLUS

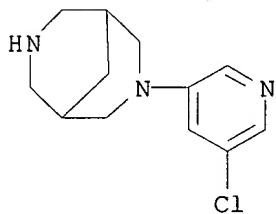
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)



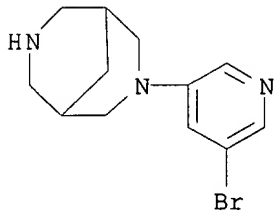
RN 345317-15-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethoxy-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 345317-16-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)

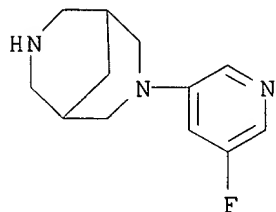


RN 345317-17-1 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-bromo-3-pyridinyl)- (9CI) (CA INDEX NAME)

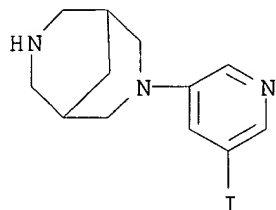


RN 345317-18-2 CAPLUS

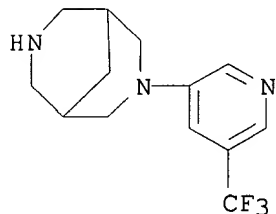
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)



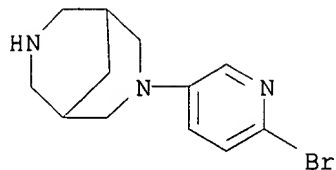
RN 345317-19-3 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-iodo-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 345317-20-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-[5-(trifluoromethyl)-3-pyridinyl]- (9CI) (CA INDEX NAME)

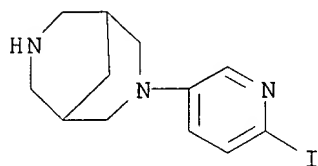


RN 345317-21-7 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-bromo-3-pyridinyl)- (9CI) (CA INDEX NAME)



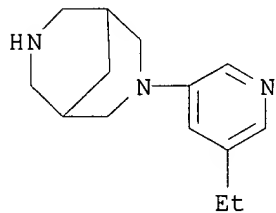
RN 345317-22-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-iodo-3-pyridinyl)- (9CI) (CA INDEX NAME)



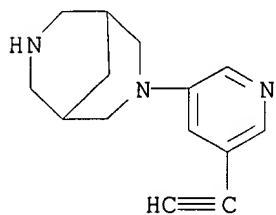
RN 345317-23-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 345317-24-0 CAPLUS

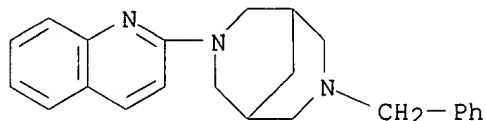
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethynyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 345317-25-1 CAPLUS

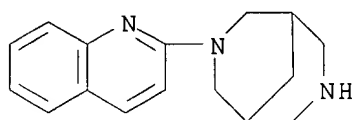
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(phenylmethyl)-7-(2-quinolinyl)- (9CI)

(CA INDEX NAME)



RN 345317-26-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(2-quinolinyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:120739 CAPLUS

DOCUMENT NUMBER: 134:326572

TITLE: Chiral bicyclic phosphoramidites - a new class of ligands for asymmetric catalysis

AUTHOR(S): Huttenloch, Oliver; Spieler, Jan; Waldmann, Herbert

CORPORATE SOURCE: Max-Planck-Institut für molekulare Physiologie
Abteilung Chemische Biologie, Dortmund, 44227,

Germany

SOURCE: Chemistry--A European Journal (2001), 7(3), 671-675
CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:326572

AB The development of new ligands for catalytic asym. C-C bond formation is of great interest to org. synthesis. The prepn. of new class of chiral phosphoramidites that embody one or two binaphthol units attached to an achiral azabicyclic [3.3.1] or [3.3.0] framework is described. These ligands were easily accessible from

(R)-1,1'-binaphthyl-2,2'-dioxaphosphor-chloridite and the corresponding heterobicyclic core. They were employed in enantioselective Cu-catalyzed addns. of different dialkylzinc reagents to cyclic and acyclic enones. The chiral ketones were obtained with an enantiomeric ratio up to 91:9. The choice of the best ligand proved to

be

strongly dependent on each substrate. In addn., ligand derived from 1,5-dimethyl-3,7-diazabicyclo[3.3.0]octane was the most suitable for Rh-catalyzed hydrogenations of .alpha.,.beta.-unsatd. esters, giving rise to di-Me 2-methylsuccinate and Me N-acetylalaninate with enantiomer

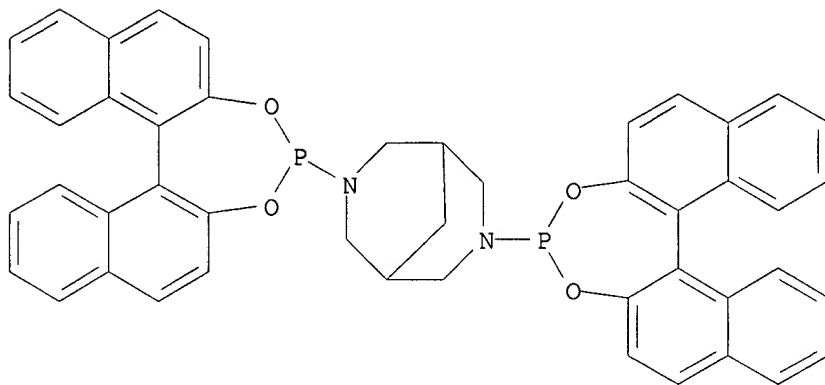
ratios

up to 95:5.

IT 335616-63-2P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);

USES (Uses)
 (prepn. of chiral bicyclic phosphoramidites as new class of ligands
 for
 asym. catalysis)
 RN 335616-63-2 CAPLUS
 CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-bis[(11bR)-dinaphtho[2,1-d:1',2'-
 f][1,3,2]dioxaphosphepin-4-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR
 THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L8 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:780169 CAPLUS
 DOCUMENT NUMBER: 134:85911
 TITLE: ¹H NMR spectral study of some 4-hydroxy-2,6-diphenylpiperidines and a systematic analysis of ¹H chemical shifts in some piperidines and 3,7-diazabicyclo[3.3.1]nonane derivatives
 AUTHOR(S): Pandiarajan, K.; Manimekalai, A.; Rajarajan, G.
 CORPORATE SOURCE: Department of Chemistry, Annamalai University, Annamalai Nagar, 608 002, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (2000), 39B(7), 517-524
 CODEN: IJSBDB; ISSN: 0376-4699
 PUBLISHER: National Institute of Science Communication, CSIR
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB ¹H NMR spectra have been recorded for some 3,5-dimethyl-2,6-diphenyl-4-piperidinol derivs. and their corresponding axial 4-hydroxy epimers. The proton chem. shifts and coupling consts. have been detd. by anal. of the spectra. The vicinal coupling consts. suggest that a boat form may make a slight contribution to the equatorial alcs. The .DELTA..delta.ea value for the protons in 5-position is less in the axial alc. than in the corresponding equatorial alc. and becomes neg. in one case. The effects

of Me, Et, iso-Pr and hydroxyl groups on the chem. shifts of the ring protons are discussed. Anal. of the chem. shifts of some 9-hydroxy-3,7-diazabicyclo[3.3.1]nonanes suggests that the 3,7-di-Ph substituted compds. exist in a boat-chair conformation.

IT 187521-32-0 187521-34-2 187800-56-2

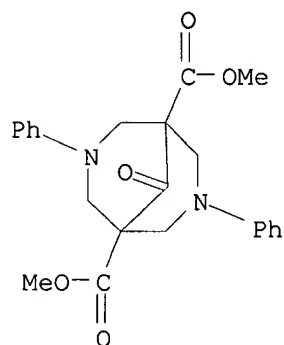
317820-65-8

RL: PRP (Properties)

(proton NMR study of some piperidinols and diazabicyclononane derivs.)

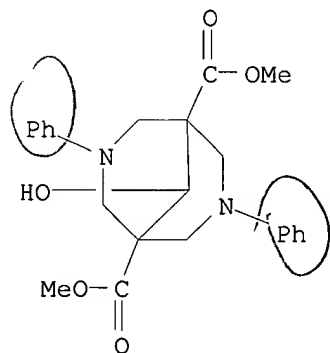
RN 187521-32-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)



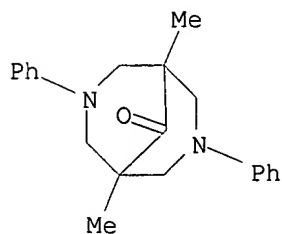
RN 187521-34-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-hydroxy-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)

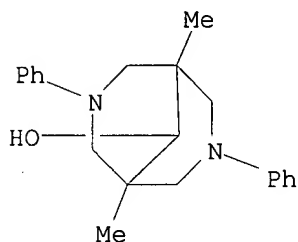


RN 187800-56-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3,7-diphenyl- (9CI) (CA INDEX NAME)



RN 317820-65-8 CAPLUS
 CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 1,5-dimethyl-3,7-diphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

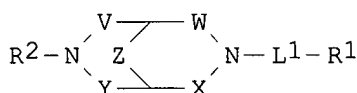
FORMAT

ANSWER 5 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:535147 CAPLUS
 DOCUMENT NUMBER: 133:135332
 TITLE: Preparation of diazabicyclic derivatives as nicotinic
 acetylcholine receptor ligands
 INVENTOR(S): Bunnelle, William H.; Cristina, Daniela Barlocco;
 Daanen, Jerome F.; Dart, Michael J.; Meyer, Michael
 D.; Ryther, Keith B.; Schrimpf, Michael R.; Sippy,
 Kevin B.; Toupence, Richard B.
 PATENT ASSIGNEE(S): Abbott Laboratories, USA
 SOURCE: PCT Int. Appl., 123 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

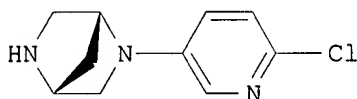
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000044755	A1	20000803	WO 2000-US1620	20000125
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,				

Hong Liu

MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
 SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ,
 BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
 DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
 CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
 EP 1147112 A1 20011024 EP 2000-906998 20000125
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO
 BR 2000007664 A 20020507 BR 2000-7664 20000125
 NO 2001003731 A 20010918 NO 2001-3731 20010730
 PRIORITY APPLN. INFO.: US 1999-239838 A 19990129
 WO 2000-US1620 W 20000125
 OTHER SOURCE(S): MARPAT 133:135332
 GI



I



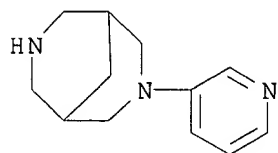
II

AB The title compds. (I) [wherein V and X = independently a bond or CH₂; W and Y = independently a bond, CH₂, or CH₂CH₂; Z = CH₂, CH₂CH₂, or CH₂CH₂CH₂; L₁ = a bond or (CH₂)_n; n = 1-5; R₁ = certain heteroarom. rings, such as pyridinyl, pyrimidinyl, pyrazinyl, quinolinyl, etc.; R₂ = H, alkoxy carbonyl, (amino)alkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy(alkyl), phenoxycarbonyl, or NH₂] and their pharmaceutically acceptable salts were prep'd. as cholinergic modulators for the treatment of pain and other conditions. For example, (-)-II.bul.Ts-OH was prep'd. in a multi-step sequence involving N-protection of (1R,4R)-2-benzyl-2,5-diazabicyclo[2.2.1]heptane.bul.2HBr with CO(OBu-t)₂ (94%), debenzylation (93%), addn. of 2-chloro-5-iodopyridine (67%), and deprotection followed by salt formation (71%). (-)-II.bul.Ts-OH exhibited high affinity for the nicotinic acetylcholine receptor with K_i of 0.01 nM and showed a significant antinociceptive effect at the minimally ED of 0.62 .mu.mol/kg in the mouse hot plate paradigm.

IT **286945-99-1P**, 3-(3-Pyridinyl)-3,7-diazabicyclo[3.3.1]nonane
286946-00-7P, 3-(6-Chloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepn. of N-substituted diazabicycloalkanes as nicotinic acetylcholine receptor ligands by addn. of haloheterocycles to protected diazabicycloalkanes followed by deprotection and optional substitution)

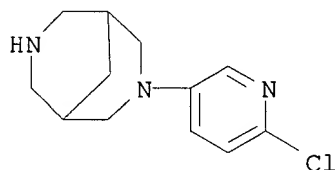
RN 286945-99-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 286946-00-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)



IT **286946-01-8P**, 3-(6-Chloro-5-methyl-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-02-9P**, 3-(5,6-Dichloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-03-0P**, 3-(6-Chloro-5-ethynyl-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-04-1P**, 3-(6-Chloro-5-cyano-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-05-2P**, 3-(5-Methoxy-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-06-3P**, 3-(6-Fluoro-5-methyl-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-07-4P**, 3-(6-Fluoro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-08-5P**, 3-(5-Ethynyl-6-fluoro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-09-6P**, 3-(5-Cyano-6-fluoro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286946-10-9P**, 3-(5-Bromo-6-chloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane **286947-18-0P**, 3-(3-Pyridinyl)-3,7-diazabicyclo[3.3.1]nonane bis(4-methylbenzenesulfonate) **286947-19-1P**, 3-(6-Chloro-3-pyridinyl)-3,7-diazabicyclo[3.3.1]nonane 4-methylbenzenesulfonate

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological

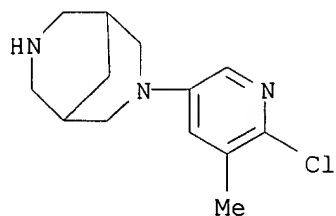
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-substituted diazabicycloalkanes as nicotinic acetylcholine

receptor ligands by addn. of haloheterocycles to protected diazabicycloalkanes followed by deprotection and optional substitution)

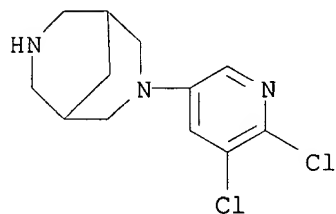
RN 286946-01-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-5-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



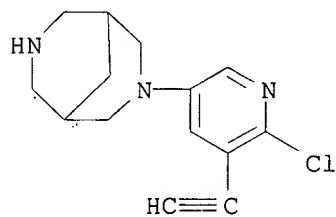
RN 286946-02-9 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5,6-dichloro-3-pyridinyl)- (9CI) (CA INDEX NAME)



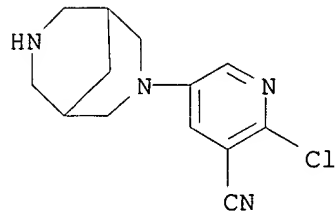
RN 286946-03-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-5-ethynyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 286946-04-1 CAPLUS

CN 3-Pyridinecarbonitrile, 2-chloro-5-(3,7-diazabicyclo[3.3.1]non-3-yl)- (9CI) (CA INDEX NAME)

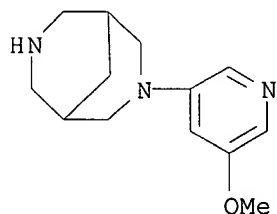


RN 286946-05-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-methoxy-3-pyridinyl)- (9CI) (CA

INDEX

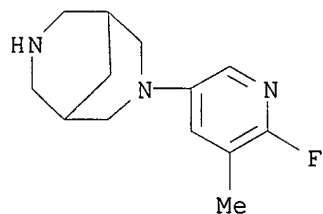
NAME)



RN 286946-06-3 CAPLUS

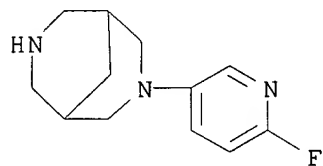
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-fluoro-5-methyl-3-pyridinyl)- (9CI)

(CA INDEX NAME)



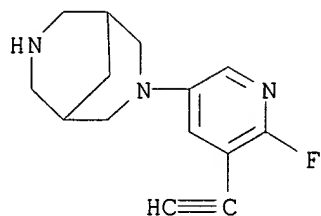
RN 286946-07-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)

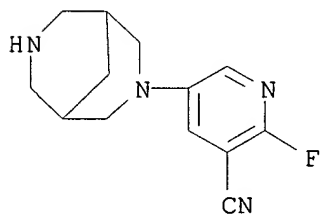


RN 286946-08-5 CAPLUS

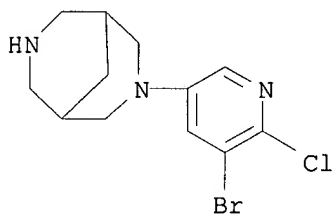
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-ethynyl-6-fluoro-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 286946-09-6 CAPLUS
CN 3-Pyridinecarbonitrile, 5-(3,7-diazabicyclo[3.3.1]non-3-yl)-2-fluoro-
(9CI) (CA INDEX NAME)



RN 286946-10-9 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(5-bromo-6-chloro-3-pyridinyl)- (9CI)
(CA INDEX NAME)

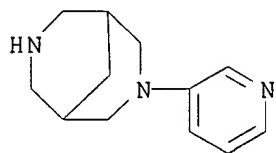


RN 286947-18-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(3-pyridinyl)-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 286945-99-1

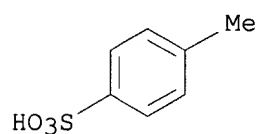
CMF C12 H17 N3



CM 2

CRN 104-15-4

CMF C7 H8 O3 S



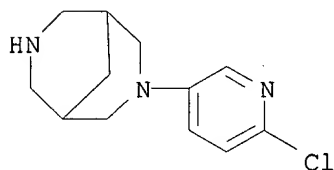
RN 286947-19-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(6-chloro-3-pyridinyl)-,
mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 286946-00-7

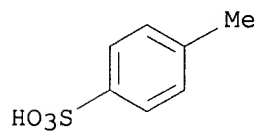
CMF C12 H16 Cl N3



CM 2

CRN 104-15-4

CMF C7 H8 O3 S



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS

Hong Liu

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L8 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:531065 CAPLUS

DOCUMENT NUMBER: 133:232367

TITLE: Diazabicyclo[3.3.1]nonanone-type ligands for the opioid receptors

AUTHOR(S): Kuhl, Ulrich; Englberger, Werner; Haurand, Michael; Holzgrabe, Ulrike

CORPORATE SOURCE: Institut fur Pharmazie und Lebensmittelchemie, Universitat Wurzburg, Wurzburg, D-97074, Germany

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000), 333(7), 226-230

CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Previously 2,4-dipyridine substituted 3,7-diazabicyclo-[3.3.1]nonanone diesters were found to have a high affinity and selectivity towards the .kappa.-opioid receptor. The purpose of this study was to check the influence of substituents at position N3 on the affinity to the .mu.-, .delta.-, and .kappa.-receptors. Whereas a phenylethyl group is able to create affinity to the .mu.-receptor, small substituents such as a hydrogen or a Me group are responsible for a high affinity to the .kappa.-receptor. In addn., a dimeric compd. was found to have affinity to the .kappa.-receptor. Although all compds. will bear at least one

pos.

charge under physiol. conditions they show a considerable lipophilicity, indicating the possibility of passing the blood-brain barrier.

IT 294181-79-6 294181-83-2 294181-86-5

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological

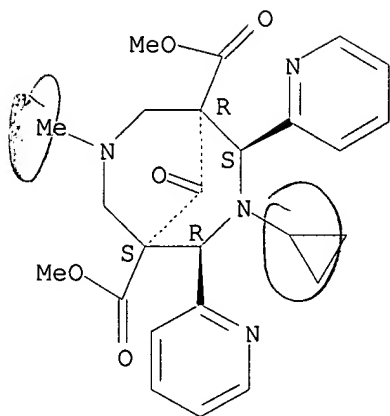
study, unclassified); PRP (Properties); BIOL (Biological study)
(diazabicyclononanone-type ligands for opioid receptors)

RN 294181-79-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 3-cyclopropyl-7-methyl-9-oxo-2,4-di-2-pyridinyl-, dimethyl ester, (1R,2S,4R,5S)-rel-
(9CI)

(CA INDEX NAME)

Relative stereochemistry.

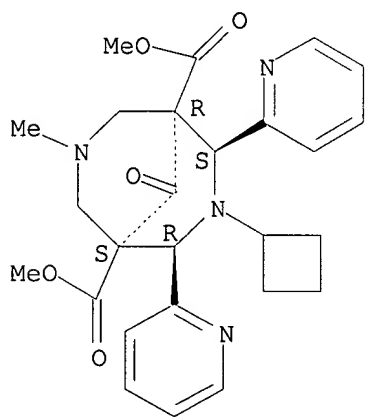


RN 294181-83-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid,
3-cyclobutyl-7-methyl-

9-oxo-2,4-di-2-pyridinyl-, dimethyl ester, (1R,2S,4R,5S)-rel- (9CI) (CA
INDEX NAME)

Relative stereochemistry.

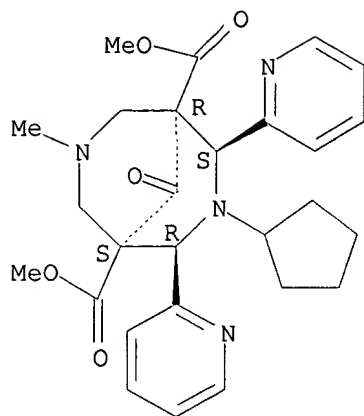


RN 294181-86-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 3-cyclopentyl-7-
methyl-9-oxo-2,4-di-2-pyridinyl-, dimethyl ester, (1R,2S,4R,5S)-rel-
(9CI)

(CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:694267 CAPLUS

DOCUMENT NUMBER: 130:66587

TITLE: Conformational Restriction of Acyclic π -Allyl
Ligands in (3,7-Diphenyl-1,5-
dimethylbispidinone)(η^3 -alkenyl)palladium
Complexes

AUTHOR(S): Gogoll, Adolf; Grennberg, Helena; Axen, Andreas
CORPORATE SOURCE: Department of Organic Chemistry, University of
Uppsala, Uppsala, 751 21, Swed.

SOURCE: Organometallics (1998), 17(24), 5248-5253
CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

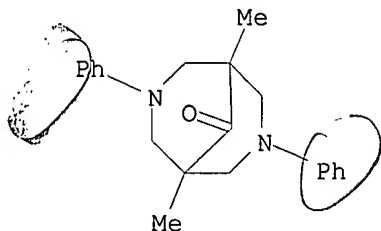
AB A chelating dinitrogen ligand based on the bispidine skeleton is shown to restrict the conformational freedom of small, acyclic π -allyl ligands in Pd complexes. The π -allyl ligand is locked into one single rotamer by entirely steric interactions. These interactions do not require the presence of bulky substituents on the π -allyl ligand. The geometry of these complexes was studied by NMR spectroscopy in combination with semiempirical calcs.

IT **187800-56-2**, 3,7-Diphenyl-1,5-dimethylbispidinone

RL: RCT (Reactant); RACT (Reactant or reagent)
(conformational restriction of acyclic π -allyl ligands in
(diphenyldimethylbispidinone)(η^3 -alkenyl)palladium complexes)

RN 187800-56-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3,7-diphenyl- (9CI) (CA
INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L8 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:484412 CAPLUS

DOCUMENT NUMBER: 129:189250

TITLE: Synthesis and conversions of polyhedral compounds.
25.

Synthesis and conversions of certain oxindole
derivatives of 1,3-diazaadamantane and
3,7-diazabicyclo[3.3.1]nonane

AUTHOR(S): Agadzhanyan, Ts. E.; Gevorkyan, K. A.

CORPORATE SOURCE: A. L. Mndzhoyan Institute of Fine Organic Chemistry,
Academy of Sciences of the Republic of Armenia,
Yerevan, 375014, Armenia

SOURCE: Chemistry of Heterocyclic Compounds (New
York) (Translation of Khimiya Geterotsiklicheskikh
Soedinenii) (1998), Volume Date 1997, 33(11),
1288-1291

PUBLISHER: CODEN: CHCCAL; ISSN: 0009-3122

DOCUMENT TYPE: Consultants Bureau

LANGUAGE: English

AB By the reaction of 1,5-dimethyl-9-oxo-3,7-diazabicyclo[3.3.1]nonane with
isatin and a no. of its derivs.,
spiro(1,3-diazaadamantane-2,3'-oxindoles)

have been synthesized. In the case of 5-bromoisatin, either
3-(3-hydroxyoxindolyl)-3,7-diazabicyclo[3.3.1]nonane or the corresponding
spirane is obtained, depending on the temp. The interaction of these
products with acetic anhydride has been studied.

IT **211917-31-6P 211917-33-8P**

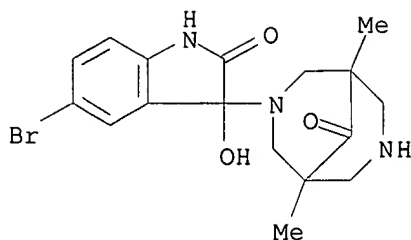
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(reactions of diazabicyclononane with isatins)

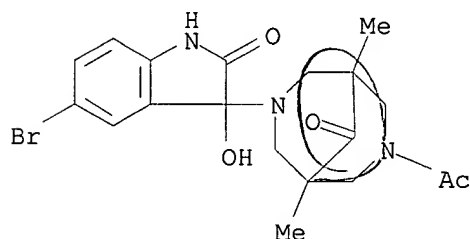
RN 211917-31-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one,

3-(5-bromo-2,3-dihydro-3-hydroxy-2-oxo-
1H-indol-3-yl)-1,5-dimethyl- (9CI) (CA INDEX NAME)

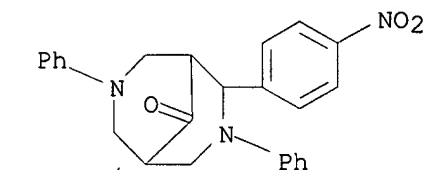


RN 211917-33-8 CAPLUS
 CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-acetyl-7-(5-bromo-2,3-dihydro-3-hydroxy-2-oxo-1H-indol-3-yl)-1,5-dimethyl- (9CI) (CA INDEX NAME)



ANSWER 9 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1997:665555 CAPLUS
 DOCUMENT NUMBER: 127:307286
 TITLE: Study on the synthesis and antibacterial activity of mannich bases containing .alpha.,.beta.-unsaturated ketone
 AUTHOR(S): Gu, Shangxiang; Yao, Kaling; Gu, Yonghong
 CORPORATE SOURCE: Dep. Chem., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China
 SOURCE: Yaoxue Xuebao (1997), 32(1), 38-42
 CODEN: YHHPAL; ISSN: 0513-4870
 PUBLISHER: Chinese Academy of Medical Sciences, Institute of Materia Media
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 AB 12 Mannich bases contg. .alpha.,.beta.-unsatd. ketone were synthesized and characterized by elemental anal., IR, ¹HNMR, UV and MS spectra. Some of the compds. showed marked antibacterial activity.
 IT 197514-66-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (study on the synthesis and antibacterial activity of mannich bases)

contg. .alpha.,.beta.-unsatd. ketone)
RN 197514-66-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 2-(4-nitrophenyl)-3,7-diphenyl- (9CI)
(CA INDEX NAME)



~~18~~ ANSWER 10 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:172468 CAPLUS

DOCUMENT NUMBER: 126:199654

TITLE: (.pi.-Allyl)palladium Complexes with
N,N'-Diphenylbispidinone Derivatives as a New Type of
Chelating Nitrogen Ligand: Complexation Studies,
Spectroscopic Properties, and an X-ray Structure of
(3,7-Diphenyl-1,5-dimethylbispidinone)[(1,3-.eta.3-
propenyl)-palladium] Trifluoromethanesulfonate
Gogoll, Adolf; Grennberg, Helena; Axen, Andreas
Department of Organic Chemistry, University of
Uppsala, Uppsala, 751 21, Swed.
SOURCE: Organometallics (1997), 16(6), 1167-1178
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:199654

AB A series of 3,7-diazabicyclo[3.3.1]nonane (bispidine) derivs. have been synthesized, and their properties as bidentate nitrogen ligands for (.pi.-allyl)palladium complexes have been investigated. Complexes of these ligands and of N,N'-diphenylpiperazine and N,N'-diphenyl-1,4-diazacyclooctane with (1,3-.eta.3-propenyl)palladium are described, in particular their effects on the proton chem. shifts of the .pi.-allyl ligand. Ligand dynamics of the complexes is discussed. The structure of [(3,7-diphenyl-1,5-dimethylbispidinone)(1,3-.eta.3-propenyl)Pd]CF₃SO₃ has been detd. by x-ray crystallog. N,N'-Diphenylbispidine derivs. show an unusually large steric interaction with the .pi.-allyl ligand, indicated by a tilt of the .pi.-allyl plane toward the N-Pd-N plane by 122.8(8).degree.. Chem. shift changes of the .pi.-allyl protons due to the arom. ring current are related to the geometry of the complexes. The ligands are tested on the larger 2-methylene-6,6-dimethylbicyclo[3.1.1]hept-2,3,10-.eta.3-enyl ligand, demonstrating their potential as chem. shift reagents.

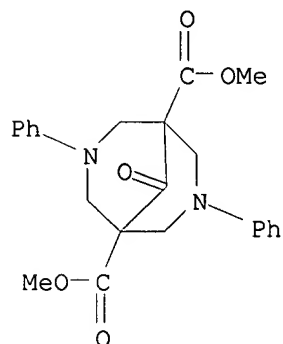
IT **187521-32-0P 187800-56-2P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

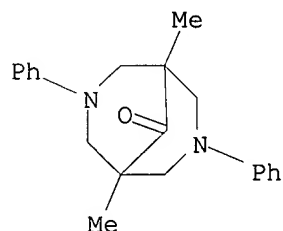
as (prepn. of allylpalladium complexes with diphenylbispidinone derivs.

new type of chelating nitrogen ligand and their complexation studies

and spectroscopic properties)
RN 187521-32-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 187800-56-2 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-dimethyl-3,7-diphenyl- (9CI) (CA INDEX NAME)



~~L8~~ ANSWER 11 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:57952 CAPLUS
DOCUMENT NUMBER: 126:185747
TITLE: Chemical shift assignment of geminal protons in 3,7-diazabicyclo[3.3.1]nonanes: an unexpected deviation from the axial/equatorial chemical shift order
AUTHOR(S): Gogoll, Adolf; Grennberg, Helena; Axen, Andreas
CORPORATE SOURCE: Department of Organic Chemistry, University of Uppsala, Uppsala, 751 21, Swed.
SOURCE: Magnetic Resonance in Chemistry (1997), 35(1), 13-20
CODEN: MRCHEG; ISSN: 0749-1581
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The chem. shift order of axial and equatorial methylene protons in 1,5-disubstituted 3,7-diazabicyclo [3.3.1] nonan-9-ones may be altered by substituents in the 1,5-positions, but the corresponding alcs. behave differently. Unambiguous signal assignments for a series of the title

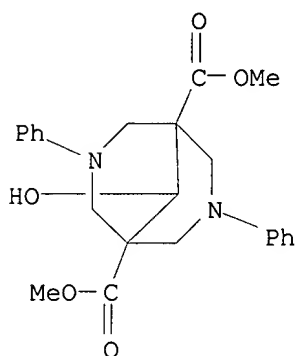
comps. are provided, based on ³JCH coupling consts. and on {¹H} ¹³C heteronuclear Overhauser effects. Substituent anisotropy effects as a source of the chem. shift changes are discussed.

IT **187521-34-2P**

RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(deviation from axial/equatorial chem. shift order and chem. shift
assignment of geminal protons in 3,7-diazabicyclo[3.3.1]nonanes)

RN 187521-34-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-hydroxy-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)

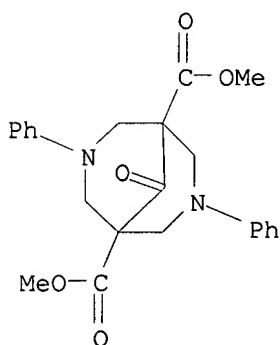


IT **187521-32-0**

RL: RCT (Reactant); RACT (Reactant or reagent)
(deviation from axial/equatorial chem. shift order and chem. shift
assignment of geminal protons in 3,7-diazabicyclo[3.3.1]nonanes)

RN 187521-32-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 9-oxo-3,7-diphenyl-, dimethyl ester (9CI) (CA INDEX NAME)



~~DB~~ ANSWER 12 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:322870 CAPLUS

DOCUMENT NUMBER: 120:322870

TITLE: Mannich reaction with arylamine as the amino

component. (X). Mannich reaction of arylamine with benzylidenebutanone

AUTHOR(S): Liao, Hongbiao; Li, Yan; Xu, Xiujuan

CORPORATE SOURCE: Dep. Chem., Beijing Normal Univ., Beijing, 100875, Peop. Rep. China

SOURCE: Beijing Shifan Daxue Xuebao, Ziran Kexueban (1992), 28(3), 367-71

CODEN: BSDKDH; ISSN: 0476-0301

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

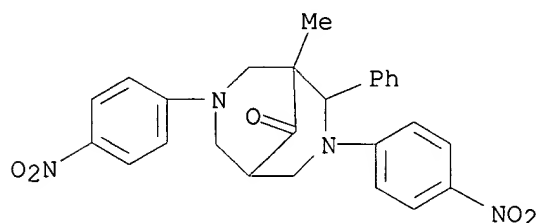
AB Mannich reaction of $\text{PhCH:CR}_1\text{COCH}_2\text{R}_2$ ($\text{R}_1, \text{R}_2 = \text{H, Me}$) with R_3NH_2 ($\text{R}_3 = \text{Ph, 4-ClC}_6\text{H}_4, 4\text{-BrC}_6\text{H}_4, 3,4\text{-Cl}_2\text{C}_6\text{H}_3, 4\text{-MeC}_6\text{H}_4, 4\text{-MeOC}_6\text{H}_4, 4\text{-methoxy-2-nitrophenyl}$) gave 60-85% $\text{PhCH:CR}_1\text{COCHR}_2\text{CH}_2\text{NHR}_3$.

IT **155498-59-2P**

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 155498-59-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1-methyl-3,7-bis(4-nitrophenyl)-2-phenyl- (9CI) (CA INDEX NAME)



18 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:118865 CAPLUS

DOCUMENT NUMBER: 112:118865

TITLE: Preparation of 3,7-diazabicyclo[3.3.1]nonanes as heat and light stabilizers

INVENTOR(S): Aumüller, Alexander; Neumann, Peter; Trauth, Hubert

PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 13 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3743279	A1	19890629	DE 1987-3743279	19871219
US 4943391	A	19900724	US 1988-286295	19881210
EP 324945	A2	19890726	EP 1988-120776	19881213
EP 324945	A3	19910116		
EP 324945	B1	19940309		
R: BE, CH, DE, FR, GB, IT, LI				
JP 01211588	A2	19890824	JP 1988-318709	19881219

PRIORITY APPLN. INFO.:

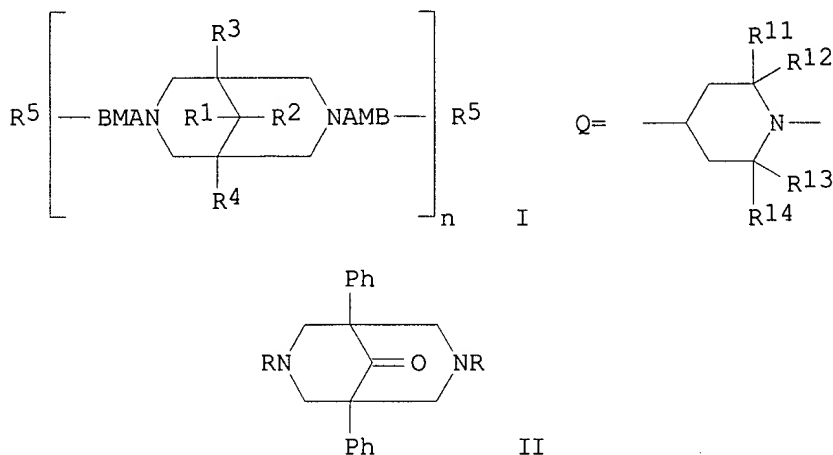
DE 1987-3743279

19871219

OTHER SOURCE(S):

CASREACT 112:118865

GI



AB The title compds. [I; A, B = bond, C1-22 alkylene, cycloalkylene, (CH₂)_mO₂, (CH₂)_mCONR₁₀, (CH₂)_mCONH(CH₂)_l; M = piperidinediyl group Q which

may be bound to A via the C- or N-atom; R₁ = H, R₂ = H, OH; R₁R₂ = O; R₃, R₄ = (un)substituted Ph, 1- or 2-naphthyl; R₅ = H, cyano, OH, alkanoyloxy,

etc.; MBR₅ = substituted hydroxyphenyl, N-attached heterocyclyl; R₁₀ = H, C1-22 alkyl, Ph, etc.; R₁₁-R₁₄ = C1-4 alkyl; R₁₁R₁₂, R₁₃R₁₄ = (CH₂)₄₋₅;

l,

m = 1-20; n = 1-70] were prepd. as heat and light stabilizers for org. materials (no data). Thus, (PhCH₂)₂CO, QH₂(R₁₁-R₁₄ = Me), and paraformaldehyde were heated 6 h in EtOH to give title compd. II (R = C-attached QH, R₁₁-R₁₄ = Me).

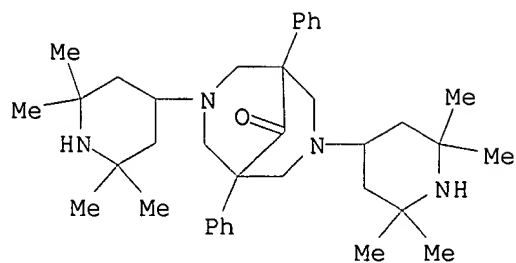
IT **124699-37-2P 124699-38-3P 124699-39-4P**

124699-40-7P 124699-41-8P 125636-30-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as heat and light stabilizer)

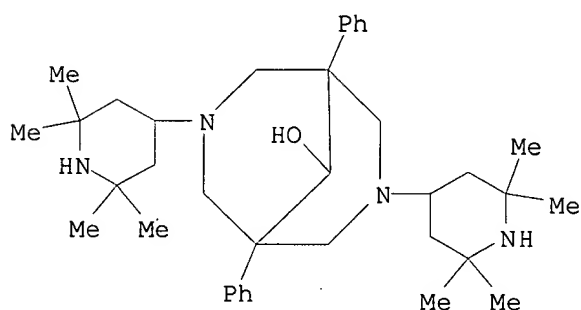
RN 124699-37-2 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-diphenyl-3,7-bis(2,2,6,6-tetramethyl-4-piperidinyl)- (9CI) (CA INDEX NAME)



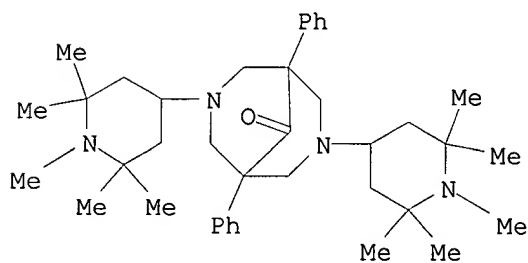
RN 124699-38-3 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 1,5-diphenyl-3,7-bis(2,2,6,6-tetramethyl-4-piperidinyl)- (9CI) (CA INDEX NAME)



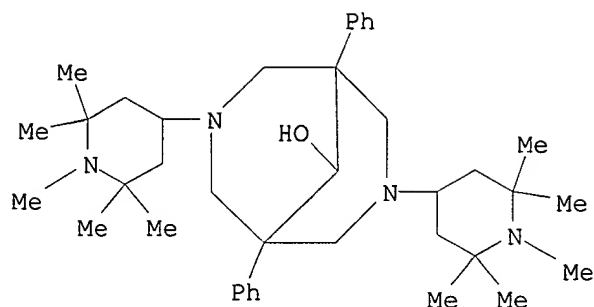
RN 124699-39-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-bis(1,2,2,6,6-pentamethyl-4-piperidinyl)-1,5-diphenyl- (9CI) (CA INDEX NAME)



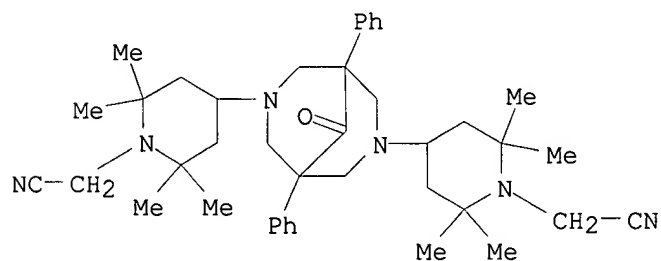
RN 124699-40-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 3,7-bis(1,2,2,6,6-pentamethyl-4-piperidinyl)-1,5-diphenyl- (9CI) (CA INDEX NAME)



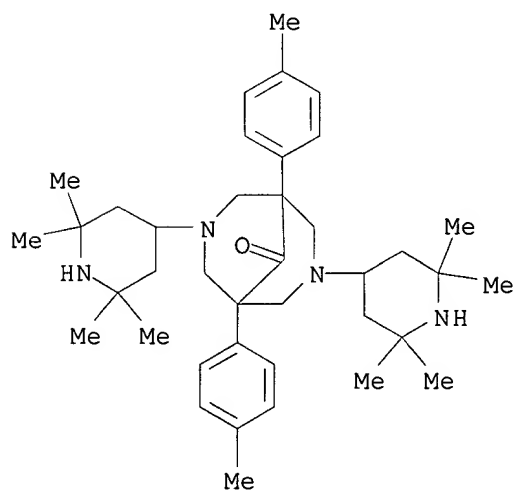
RN 124699-41-8 CAPLUS

CN 1-Piperidineacetonitrile, 4,4'-(9-oxo-1,5-diphenyl-3,7-diazabicyclo[3.3.1]nonane-3,7-diyl)bis[2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



RN 125636-30-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,5-bis(4-methylphenyl)-3,7-bis(2,2,6,6-tetramethyl-4-piperidinyl)- (9CI) (CA INDEX NAME)

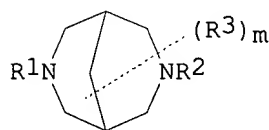


L8 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2002 ACS
 X ACCESSION NUMBER: 1989:415252 CAPLUS
 DOCUMENT NUMBER: 111:15252
 TITLE: Improving the lightfastness of colored organic materials
 INVENTOR(S): Kaneko, Yutaka
 PATENT ASSIGNEE(S): Konica Co., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

lost reference

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
JP 63281158	A2	19881117	JP 1987-116326	19870513

GI



AB In the title method, an org. colored material and I [R1, R2 = H, alkyl, cycloalkyl, alkenyl, cycloalkenyl, alkynyl, aryl, heterocyclyl, acyl, sulfonyl, carbamoyl, phosphonyl, sulfamoyl, oxycarbonyl; R3 = substituent;

m = 0-6] are allowed to coexist. The method is esp. useful in color photog., inks and fabric dyes. A photog material contained I [R1 = CH3; R2 = C6H5CH2] and a magenta dye to prevent photofading.

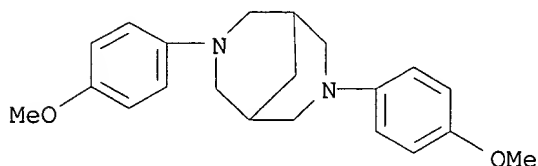
IT 121171-68-4 121171-69-5 121171-70-8
 121171-72-0 121171-73-1 121171-76-4
 121185-53-3

RL: USES (Uses)

(lightfastness improvement additive, for orgs.)

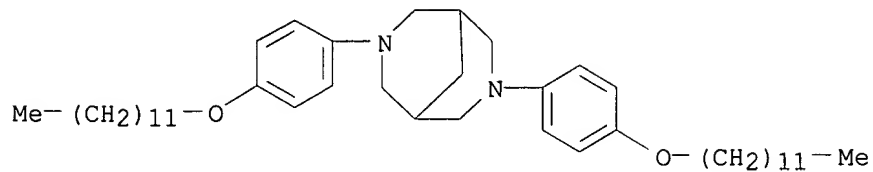
RN 121171-68-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



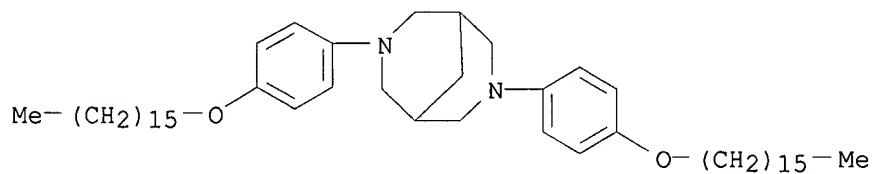
RN 121171-69-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-bis[4-(dodecyloxy)phenyl]- (9CI) (CA INDEX NAME)



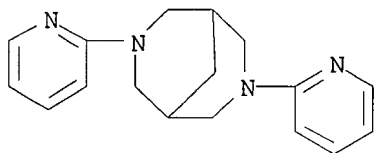
RN 121171-70-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-bis[4-(hexadecyloxy)phenyl]- (9CI)
(CA INDEX NAME)



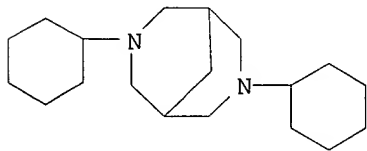
RN 121171-72-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-di-2-pyridinyl- (9CI) (CA INDEX NAME)



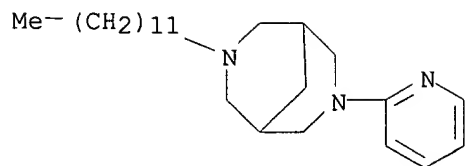
RN 121171-73-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-dicyclohexyl- (9CI) (CA INDEX NAME)

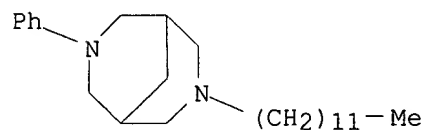


RN 121171-76-4 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-dodecyl-7-(2-pyridinyl)- (9CI) (CA INDEX NAME)

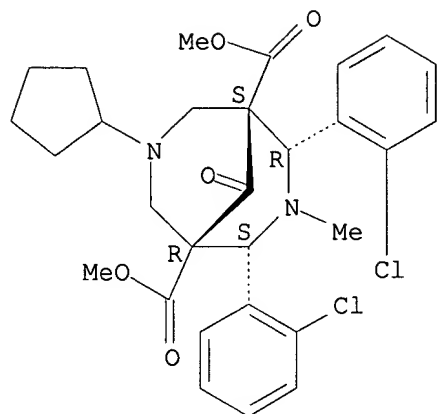


RN 121185-53-3 CAPLUS
 CN 3,7-Diazabicyclo[3.3.1]nonane, 3-dodecyl-7-phenyl- (9CI) (CA INDEX NAME)



ANSWER 15 OF 28 CAPLUS COPYRIGHT 2002 ACS
 X
 ACCESSION NUMBER: 1985:470647 CAPLUS
 DOCUMENT NUMBER: 103:70647
 TITLE: Synthesis and conformational study of
 3,7-diazabicyclo[3.3.1]nonan-9-ones
 AUTHOR(S): Caujolle, Raymond; Castera, Pierre; Lattes, Armand
 CORPORATE SOURCE: Lab. Chim. Ther., Toulouse, 31077, Fr.
 SOURCE: Bull. Soc. Chim. Fr. (1984), (9-10, Pt. 2), 413-16
 CODEN: BSCFAS; ISSN: 0037-8968
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 AB ¹H and ¹³C NMR studies of various 3,7-diazabicyclo [3.3.1]nonanones
 indicate an equil. between chair-chair and chair-boat conformations for
 these compds. N(7) atom bears bulky substituents, the chair-boat form is
 more favored at equil.
 IT 97564-84-6 97564-85-7 97564-86-8
 97564-87-9 97564-89-1
 RL: PRP (Properties)
 (carbon-13 and proton NMR of, conformation in relation to)
 RN 97564-84-6 CAPLUS
 CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-
 chlorophenyl)-7-cyclopentyl-3-methyl-9-oxo-, dimethyl ester, (endo,endo)-
 (9CI) (CA INDEX NAME)

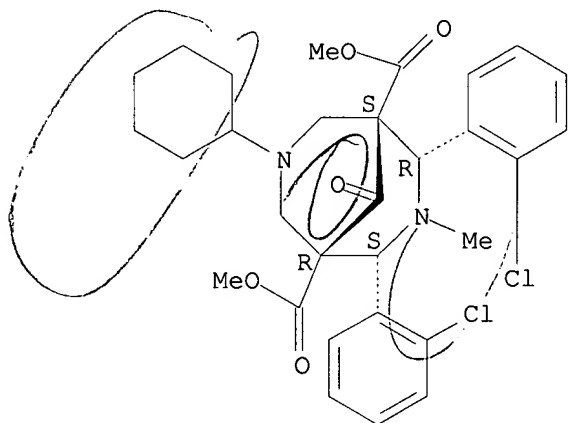
Relative stereochemistry.



RN 97564-85-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-chlorophenyl)-7-cyclohexyl-3-methyl-9-oxo-, dimethyl ester, (endo,endo)-(9CI) (CA INDEX NAME)

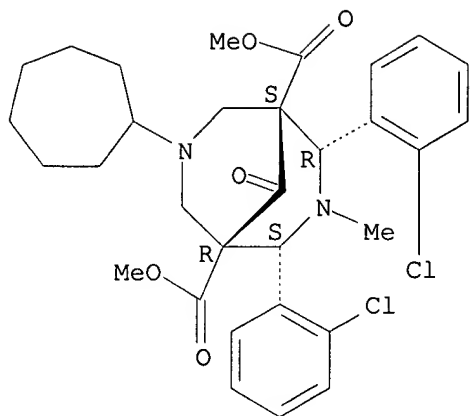
Relative stereochemistry.



RN 97564-86-8 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-chlorophenyl)-7-cycloheptyl-3-methyl-9-oxo-, dimethyl ester, (endo,endo)-(9CI) (CA INDEX NAME)

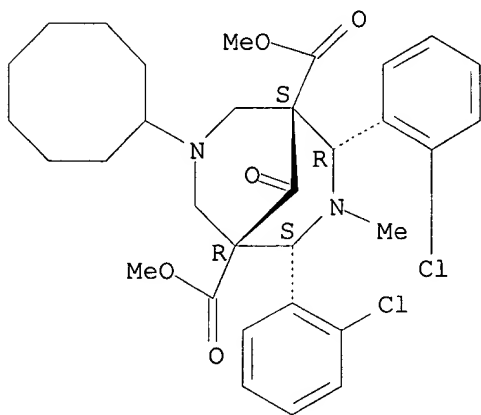
Relative stereochemistry.



RN 97564-87-9 CAPLUS

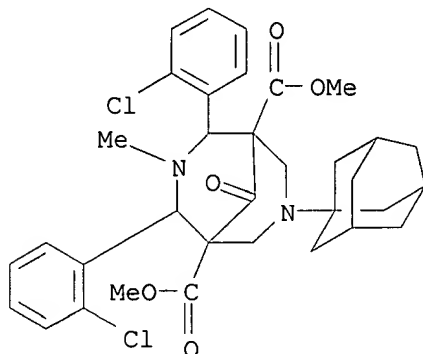
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-chlorophenyl)-7-cyclooctyl-3-methyl-9-oxo-, dimethyl ester, (endo,endo)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

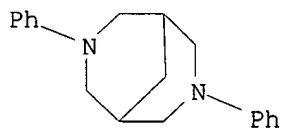


RN 97564-89-1 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 2,4-bis(2-chlorophenyl)-3-methyl-9-oxo-7-tricyclo[3.3.1.13,7]dec-1-yl-, dimethyl ester, (endo,endo)-(9CI) (CA INDEX NAME)

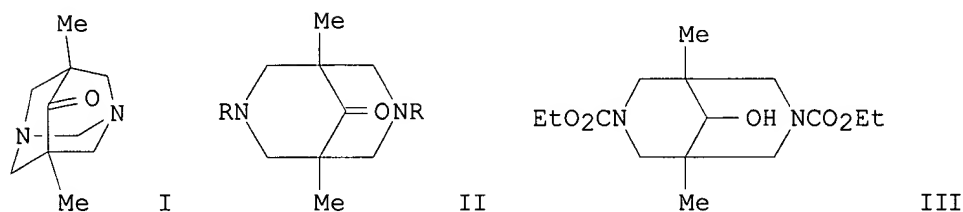


18 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1984:581621 CAPLUS
 DOCUMENT NUMBER: 101:181621
 TITLE: Crystal and molecular structure of
 3,7-diphenyl-3,7-diazabicyclo[3.3.1]nonane, C₁₉H₂₂N₂
 AUTHOR(S): Levina, O. I.; Potekhin, K. A.; Kurkutova, E. N.;
 Struchkov, Yu. T.; Palyulin, V. A.; Zefirov, N. S.
 CORPORATE SOURCE: Vladimir. Pedagog. Inst., Vladimir, USSR
 SOURCE: Dokl. Akad. Nauk SSSR (1984), 277(2), 367-70
 [Crystallogr.]
 CODEN: DANKAS; ISSN: 0002-3264
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 AB The title compd. is monoclinic, space group P2₁/c, with a 10.060(1), b
 17.338(2), c 9.123(2) .ANG., and .beta. 100.62(1).degree.; Z = 4. The
 at. parameters are given. The structure was detd. by direct methods and
 refined by full-matrix least-squares to R = 0.074. The mol. has the
 double-chain conformation.
 IT **54171-89-0**
 RL: PRP (Properties)
 (structure of)
 RN 54171-89-0 CAPLUS
 CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)



18 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1982:104172 CAPLUS
 DOCUMENT NUMBER: 96:104172
 TITLE: Synthesis and reactions of polyhedral compounds. II.

and
 Synthesis of 5,7-dimethyl-1,3-diazaadamantan-6-one
 -6-ol and their conversion into 3,7-
 diacyl(dicarbalkoxy, diarylsulfonyl)-3,7-
 diazabicyclo[3,3,1]nonanes
 AUTHOR(S): Agadzhanyan, Ts. E.; Arutyunyan, G. L.
 CORPORATE SOURCE: Inst. Tonkoi Org. Khim. im. Mndzhoyana, Yerevan, USSR
 SOURCE: Arm. Khim. Zh. (1981), 34(11), 963-8
 CODEN: AYKZAN; ISSN: 0515-9628
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



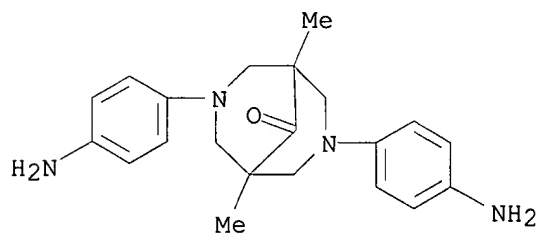
AB Cyclocondensation of EtCOEt, HCHO, and AcONH₄ gave 19.5% I, which reacted with RCOCl, RO₂CCl, or ArSO₂Cl to give II [R = BrCH₂CO, BrCH₂CH₂CO, CH₂:CHCO, Bz, (phthalimidomethoxy)carbonyl, EtOCO, PhCH₂OCO, 4-MeC₆H₄SO₂, 4-(MeO₂CNH)C₆H₄SO₂]. LiAlH₄ redn. of I gave 83.3% alc., which with ClCO₂Et gave III.

IT **80808-97-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 80808-97-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-bis(4-aminophenyl)-1,5-dimethyl-
 (9CI) (CA INDEX NAME)



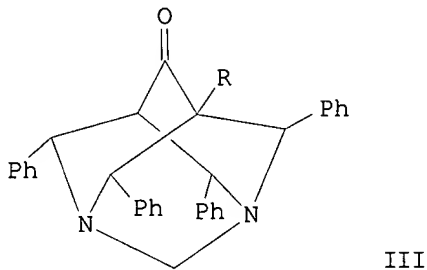
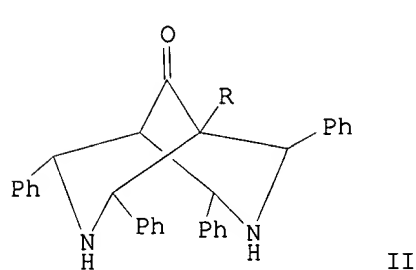
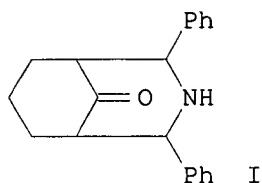
~~18~~ ANSWER 18 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1981:425025 CAPLUS

DOCUMENT NUMBER: 95:25025

TITLE: Synthesis and reactions of ketones of 3-aza-,
 3,7-diazabicyclononane and 3,7-diazaadamantane series

AUTHOR(S): Omarov, T. T.; Baisalbaeva, S. A.; Gubasheva, A. Sh.
 CORPORATE SOURCE: USSR
 SOURCE: Tr. Inst. Khim. Nauk, Akad. Nauk Kaz. SSR (1980), 52, 147-70
 CODEN: TIKNAG; ISSN: 0568-5087
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 GI



AB Condensation of cyclohexanone with BzH and H₄NOAc gave a mixt. of diazabicyclononanone I and 2,6-dibenzylidenecyclohexanone. I was methylated. The diazabicyclononanones II (R = H, Me) were obtained by a similar condensation from the resp. piperidinone. The diazaadamantanes III were obtained from II by condensation with HCHO. III were reduced to alcs. I was converted to acetylenic alcs. Addnl. reactions of I, II and III were discussed. The conformation, spectra and biol. activity of I,

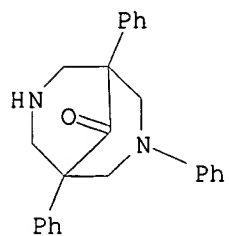
II and III were discussed with 72 refs.

IT **77446-47-0P 77446-50-5P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and spectra of)

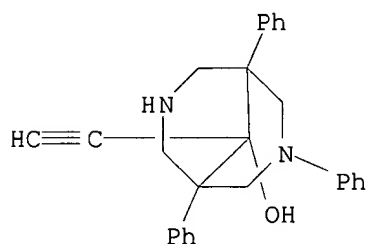
RN 77446-47-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 1,3,5-triphenyl- (9CI) (CA INDEX NAME)

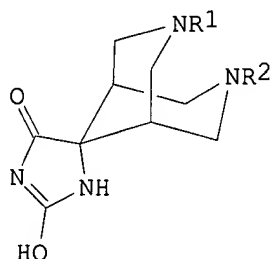
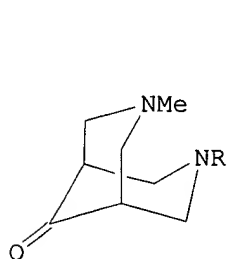


RN 77446-50-5 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-ol, 9-ethynyl-1,3,5-triphenyl- (9CI) (CA INDEX NAME)



~~18~~ ANSWER 19 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1980:426411 CAPLUS
 DOCUMENT NUMBER: 93:26411
 TITLE: Spiro heterocyclic derivatives. XV. Some N-methyl-N'-alkyl(or aralkyl)-3,7-diazabicyclo[3.3.1]nonan-9-ones and some 9-spiro-5'-hydantoin derivatives of 3,7-diazabicyclo[3.3.1]nonanes
 AUTHOR(S): Gonzalez Trigo, G.; Galvez Ruano, E.; Menendez Aguirre, C.
 CORPORATE SOURCE: Fac. Farm., Univ. Complutense Madrid, Madrid, Spain
 SOURCE: An. Quim. (1979), 75(12), 894-8
 CODEN: ANQUBU; ISSN: 0365-4990
 DOCUMENT TYPE: Journal
 LANGUAGE: Spanish
 GI



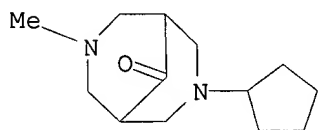
Hong Liu

AB Reaction of N-methyl-4-piperidone with HCHO and amines RNH₂ in AcOH soln. gave the 3,7-diazabicyclo[3.3.1]nonan-9-ones I [R = C1-C4 alkyl, cyclopentyl, cyclohexyl, PhCH₂, PhCH₂CH₂, Me₂N(CH₂)₃, HOCH₂CH₂], which reacted with KCN and (NH₄)₂CO₃ to give the spirohydantoins II (R₁ = Me, R₂ = R or R₁ = R, R₂ = Me). IR band of I and II and NMR chem. shifts of II are tabulated.

IT **73977-30-7P 73990-91-7P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and IR spectrum of)

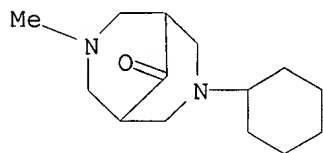
RN 73977-30-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclopentyl-7-methyl- (9CI) (CA INDEX NAME)



RN 73990-91-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclohexyl-7-methyl- (9CI) (CA INDEX NAME)



L8) ANSWER 20 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1977:601499 CAPLUS

DOCUMENT NUMBER: 87:201499

TITLE: Nonsymmetric N-substituted bispidine
 (3,7-diazabicyclo[3.3.1]nonane. I

AUTHOR(S): Hoerlein, Ulrich

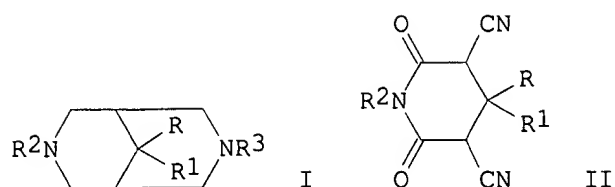
CORPORATE SOURCE: Chem. Wiss. Lab. Pharma, Bayer A.-G., Wuppertal, Ger.

SOURCE: Eur. J. Med. Chem. - Chim. Ther. (1977), 12(4), 301-5
 CODEN: EJMCA5

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



AB Bispidine derivs. I [R = R1 = Me, RR1 = (CH2)5, R2 = Me, Et, CH2Ph, R3 = H; RR1 = (CH2)4, R2 = Me, Et, R3 = H] were prepd. by condensing RR1C:C(CN)CO2Et with R2NHCOCH2CN, hydrolyzing II, and reducing diimides with LiAlH4. I [R3 = acyl, 4-FC6H4CO(CH2)3, 8-chloro-10,11-dihydrobenzo[b,f]thiepin-10-yl] were prepd. by substitution of I (R3 = H).

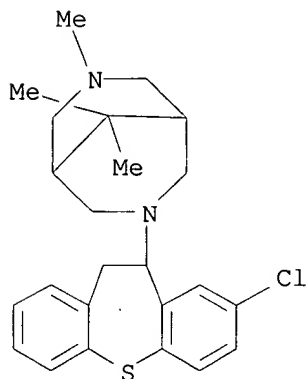
I [RR1 = (CH2)5, (CH2)4, R2 = Me, R3 = COCH2Ph] had analgesic activities of the same magnitude as morphine. Some other I exhibited various pharmacol. activity, but only to a degree.

IT **64729-96-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

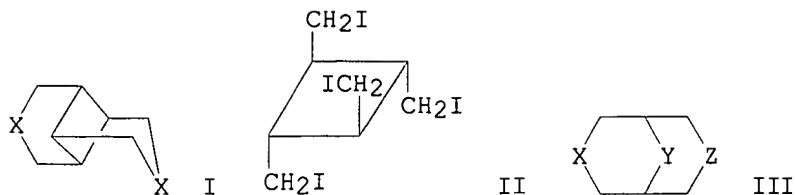
RN 64729-96-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3-(8-chloro-10,11-dihydrodibenzo[b,f]thiepin-10-yl)-7,9,9-trimethyl- (9CI) (CA INDEX NAME)



~~DB~~ ANSWER 21 OF 28 CAPLUS COPYRIGHT 2002 ACS
 X ACCESSION NUMBER: 1977:484859 CAPLUS
 DOCUMENT NUMBER: 87:84859
 TITLE: Synthesis of 4,9-diheterotricyclo[4.4.0.02,7]decanes and bicyclo[3.3.1]nonanes
 AUTHOR(S): Zefirov, N. S.; Rogozina, S. V.
 CORPORATE SOURCE: Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR
 SOURCE: Strukt. Svoistva Krist. (1974), 1, 94-9
 CODEN: SSKRDM
 DOCUMENT TYPE: Journal

LANGUAGE: Russian
GI



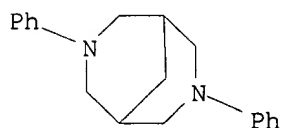
AB Tricyclodecane I (X = S) was obtained in 60% yield by refluxing II with Na₂S in abs. alc. 6 h. Analogously II refluxed with PhNH₂ 60 h in PhMe gave I (X = NPh). Bicyclononanes III (X = O, Y = O, S, Z = S; X = S, Y = O, Z = S, Se) were obtained in 1.0-18.8% yields by treatment of a bis(iodomethyl)dioxane, oxathiane with Na₂S or with Se. Addnl. obtained was 73.7% III (X = Z = NPh, Y = CH₂).

IT **54171-89-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 54171-89-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)



~~28~~ ANSWER 22 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:90040 CAPLUS

DOCUMENT NUMBER: 84:90040

TITLE: Synthesis of 4,9-diheterotricyclo[4.4.0.0^{2,7}]decenes and bicyclo[3.3.1]nonanes

AUTHOR(S): Zefirov, N. S.; Rogozina, S. V.

CORPORATE SOURCE: USSR

SOURCE: Struktura i Svoistva Kristallov (1974), (1), 94-9
From: Ref. Zh., Khim. 1975, Abstr. No. 19ZH312

DOCUMENT TYPE: Journal

LANGUAGE: Russian

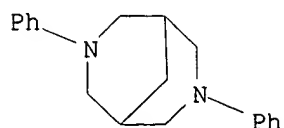
AB Title only translated.

IT **54171-89-0P**

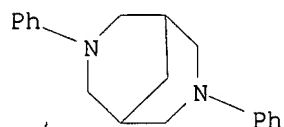
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 54171-89-0 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)

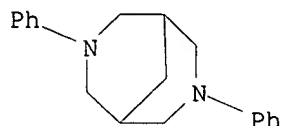


~~L8~~ ANSWER 23 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1976:52620 CAPLUS
DOCUMENT NUMBER: 84:52620
TITLE: Crystallographic data of the compounds,
N,N-diphenyl-3,7-diazabicyclo[3,3,1]nonane (C19H22N2)
and C22H20N2O2
AUTHOR(S): Levina, O. I.
CORPORATE SOURCE: USSR
SOURCE: Struktura I Svoistva Kristallov (1974), (1), 112-13
From: Ref. Zh., Khim. 1975, Abstr. No. 15B544
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Title only translated.
IT **54171-89-0**
RL: PRP (Properties)
(crystal structure of)
RN 54171-89-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)

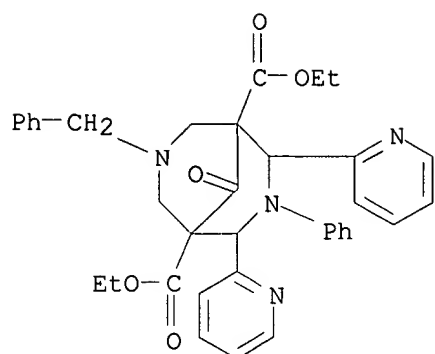


~~L8~~ ANSWER 24 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:57412 CAPLUS
DOCUMENT NUMBER: 82:57412
TITLE: Stereochemical studies. XVIII. Conformational study
of heteroanalogs of bicyclo[3.3.1]nonane
AUTHOR(S): Zefirov, N. S.; Rogozina, S. V.
CORPORATE SOURCE: Chem. Dep., Moscow State Univ., Moscow, USSR
SOURCE: Tetrahedron (1974), 30(15), 2345-52
CODEN: TETRAB
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The conformations of the heteroanalogs I thru X of bicyclo[3.3.1]nonane
were detd. from their NMR. The double chair is the preferred
conformation
for I thru V; O-O and O-S repulsions distorted the chair giving flattened
wings. VI, IX, and X had increased proportions of boat-chair forms.
IT **54171-89-0**

RL: PRP (Properties)
(conformation of, NMR in relation to)
RN 54171-89-0 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane, 3,7-diphenyl- (9CI) (CA INDEX NAME)



~~18~~ ANSWER 25 OF 28 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1969:101290 CAPLUS
DOCUMENT NUMBER: 70:101290
TITLE: Metal chelates of (2-pyridyl)-substituted
3,7-diazabicyclo[3.3.1]nonanones
AUTHOR(S): Haller, Rolf
CORPORATE SOURCE: Pharm. Inst., Univ. Freiburg/Br., Freiburg/Br., Ger.
SOURCE: Arch. Pharm. (Weinheim) (1969), 302(2), 113-18
CODEN: APBDAJ
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Hot alc. L reacts with an equal molar quant. of alc. transition metal
salt
to give MLX2 (M, X, R, R1, yield (%), m.p. (decompn.) given): Fe, SCN,
Me,
CH2Ph, 89, -; Co, SCN, Me, CH2Ph, 74, 210-12.degree.; Cd, SCN, Me, CH2Ph,
69, 180.degree.; Ni, SCN, Et, CH2Ph, 76, 212-15.degree.; Mn, Cl, Et, Me,
71, 242.degree.. The ir spectra studied indicate that the azabicyclic
complexes contain tetradentate ligands.
IT **4728-47-6**
RL: PRP (Properties)
(spectrum of, ir)
RN 4728-47-6 CAPLUS
CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-benzyl-9-oxo-3-
phenyl-2,4-di-2-pyridyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME)



L8 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1966:35818 CAPLUS

DOCUMENT NUMBER: 64:35818

ORIGINAL REFERENCE NO.: 64:6629c-h, 6630c-f

TITLE: Substituted 3,7-diaza- and 3-oxa-7-azabicyclo [3.3.1] nonanones

AUTHOR(S): Haller, R.

CORPORATE SOURCE: Univ. Freiburg/Br., Germany

SOURCE: Arzneimittelforsch. (1965), 15(11), 1327-30

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Substituted piperidones and tetrahydropyrones having active H groups in the 3,5-positions underwent a Mannich-type reaction with HCHO and a primary amine to form the title compds. Methyl or ethyl esters of 2,6-disubstituted-4-piperidone-3,5-dicarboxylic acid (CA 60, 15824a), (0.01 mole) were dissolved in hot EtOH, and a 20% excess of aq. HCHO, and the amine added in order, followed by an addnl. 100 ml. EtOH to effect complete soln. After standing several days, the insol. products were filtered off, or the sol. products obtained as residues, and crystd. The following I were prepd. [R2, R3, R4, % yield, m.p. (solvent) given]: Me, H, PhCH2 (Ia), 70, 184-5.degree. (MeOH); Et, H, PhCH2, 68.5,

161-2.degree.

(EtOH); Me, H, Me, 68, 165.degree. (MeOH-H2O, 1:2); Et, H, Me, 35, 137.degree. (EtOH-ligroine, 1:1); Et, Me, Me, 41, 158.degree. (EtOH); Me, (CH2)2OH, PhCH2, 31, 197.degree. (MeOH); Et, (CH2)2OH, PhCH2, 22, 180.degree. (EtOH-H2O, 1:1); Et, PhCH2, PhCH2, 36, 188.degree. (EtOH);

Et,

Ph, PhCH2, 76, 178.degree. (EtOH); Et, H, 2-pyridylmethyl, 73, 169-70.degree. (EtOH-H2O, 1:1). II prepd. were (identification same as for I): Me, H, Me, 55.5, 154-5.degree. (EtOH-H2O, 1:1); Me, H, PhCH2, 60.5, 183.degree. (MeOH-H2O, 4:1). III, 1,5-dicarbethoxy-7-benzyl-2,4-di(3-pyridyl)-3,7-diazabicyclo[3.3.1]nonan-9-one, 75%, m. 183.degree. (EtOH), was similarly prepd. A soln. of 10.7 g. pyridine-2-carboxaldehyde, and 4 g. 2-aminoethanol in 30 ml. MeOH was treated with 8.7 g. diethyl acetonedicarboxylate, 20 ml. ether was added, and the

mixt.

kept 1 day to give 67% diethyl 1-(2-hydroxyethyl)-2,6-di(2-pyridyl)-4-

piperidone-3,5-dicarboxylate (IV) 67%, m. 146.degree. (decompn.) (MeOH). The corresponding diethyl ester (V) (53), m. 113-14.degree. (decompn.) (EtOH-H₂O, 1:1), was similarly prepd. as was 87.5% diethyl 1-phenyl-2,6-di(2-pyridyl)-4-piperidone-3,5-dicarboxylate (VI), m. 139.degree. (decompn.) (EtOH), using aniline in place of 2-aminoethanol. IV-VI gave an intense red-violet color with alc. FeCl₃. Diethyl 2,6-di(2-pyridyl)-4-piperidone-3,5-dicarboxylate (loc. cit.) (2 g.), was acetylated with 1.5 g. AcCl in 60 ml. benzene in the presence of 2 g. CaCO₃ to yield 90% diethyl 1-acetyl-2,6-di(2-pyridyl)-4-piperidone-3,5-dicarboxylate (VII), m. 126.degree. (decompn.) (EtOH-H₂O). VII (5 millimoles) was treated with HCHO and amines in a manner similar to the prepn. of I-III to yield

7-substituted-1,5-dicarbethoxy-2,4-di(2-pyridyl)-3-acetyl-3,7-diazabicyclo [3.3.1] nonan-9-ones (VIII) as follows [R₄, % yield, m.p. (solvent) given]: H, 45, 197.degree. (decompn.) (EtOH-H₂O, 2:1); Me, 53, 130.degree. (decompn.) (EtOH-H₂O, 2:1); PhCH₂, 70, 170.degree. (decompn.) (EtOH). Esters of

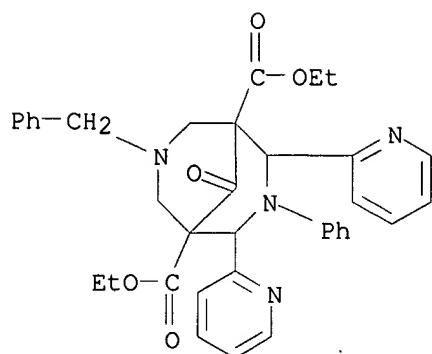
2,6-diphenyltetrahydro-4-pyrone-3,5-dicarboxylic acid (0.01 mole), were treated with HCHO and amines in the same manner as for I-III to form derivs. (IX) of

2,4-diphenyl-3-oxa-7-azabicyclo[3.3.1]nonan-9-one. IX prepds. were [R₁, R₂, % yield, m.p. (EtOH) given]: Et, allyl, 72, 131-2.degree.; Et, PhCH₂, 57, 129.degree.; Me, 2-pyridylmethyl, 54, 181-3.degree.; Et, 2-pyridylmethyl, 49, 161.degree.. Derivs. (X) of 2,4-di(2-pyridyl)-3-thia-7-azabicyclo[3.3.1]nonan-9-one were similarly prepd., starting with the Me or Et esters of 1-thia-2,6-di(2-pyridyl)cyclohexan-4-one-3,5-dicarboxylic acid (CA 63, 5613h). X prepds. (identification same as IX) were: Me, 2-pyridylmethyl, 37, 185.degree. (decompn.) (EtOH-H₂O, 2:1); Et, 2-pyridylmethyl, 35, 193.degree. (decompn.) (EtOH-H₂O, 2:1). A soln. of 0.7 g. Co(NO₃)₂·6H₂O in 20 ml. EtOH was added to a hot soln. of Ia in 40 ml. EtOH and the mixt. heated 10 min. on a steam bath; the pptd. Co chelate was only slightly sol. in H₂O, practically insol. in org. solvents, dimethylformamide, and dimethyl sulfoxide, decompd. 230-5.degree., yield 70%. A hot soln. of 0.6 g. KSCN and 0.6 g. MnCl₂·4H₂O in 30 ml. EtOH was heated on a steam bath; the pptd. KCl was filtered off, and the soln. mixed with 1 g. Ia in 40 ml. EtOH, and heated 5 min. After several hrs. standing, yellow-gold crystals of the Ia-Mn-(SCN)₂ chelate pptd., 82%, decompd. 185.degree. Am. 200.degree.. IV-VI were characterized by ir spectra as enol forms; the structures of the I-III series of compds. were confirmed by N.M.R.

IT **4728-47-6**, 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-benzyl-9-oxo-3-phenyl-2,4-di-2-pyridyl-, diethyl ester (prepn. of)

RN 4728-47-6 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonane-1,5-dicarboxylic acid, 7-benzyl-9-oxo-3-phenyl-2,4-di-2-pyridyl-, diethyl ester (7CI, 8CI) (CA INDEX NAME)



18 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1965:480662 CAPLUS

DOCUMENT NUMBER: 63:80662

ORIGINAL REFERENCE NO.: 63:14864a-e

TITLE: Synthesis of 1,5-diphenylbispidin-9-ones. VIII.
1,5-Diphenyl-3,7-dialkylbispidin-9-ones.
Asymmetrically substituted derivatives

AUTHOR(S): Chiavarelli, S.; Toeffler, H. F.; Fennoy, L. V.;
Landi-Vittory, R.; Mazzeo, P.

CORPORATE SOURCE: Ist. Super. Sanita, Rome

SOURCE: Farmaco (Pavia), Ed. Sci. (1965), 20(6), 408-20

DOCUMENT TYPE: Journal

LANGUAGE: Italian

GI For diagram(s), see printed CA Issue.

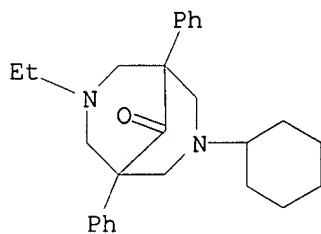
AB A series of asym. substituted 1,5-diphenyl-3,7-dialkylbispidin-9-ones (I) was prepd. from 1,3-diphenylacetone (II), paraformaldehyde (III), and acetates of primary alkylamines. An alc. soln. of 0.1 mole II, 0.4 mole III, 0.1 mole RNH₂.AcOH, and 0.1 mole R'NH₂.AcOH was refluxed 6-16 hrs., according to the employed amine. The reaction mixt. was cooled, dild. with an equal vol. H₂O, alkalized to pH 8 with 20% Na₂CO₃, kept overnight,

filtered, and the ppt. crystd. if solid, or purified through the perchlorate, if liquid. The reaction product consisted of a mixt. of sym.

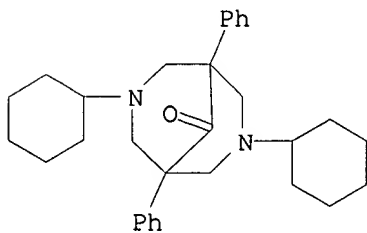
and asym. substituted I, not separable by crystn., but only by thin layer chromatography. The following I were prepd. and crystd. after chromatographic sepn. (R, R', m.p., and % yield given): Et, cyclohexyl, 132-3.degree., 43; Me, PhCH₂, 132-4.degree., 48; Et, PhCH₂, 129-31.degree., 44; Et, Ph(CH₂)₂, 131-3.degree., 50; Me, Et, 116-18.degree., 57; Et, Pr, 106-8.degree., 47; Et, iso-Pr, 140-2.degree., 41; Pr, iso-Pr, 126-8.degree., 37; Me, iso-Pr, 111-113.degree., 34. Rf and ir spectra of all the compds. are recorded. IX. 1,5-Diphenyl-3,7bis(hydroxyalkyl)- and 1,5-diphenyl-3,7-bis(methoxyalkyl)bispidin-9-ones, symmetric and asymmetric. S. Chiavarelli, H. F. Toeffler, R. Landi-Vittory, and P. Mazzeo. Ibid. 421-7. Sym. and asym. 1,5-diphenyl-3,7-bis(hydroxyalkyl)- and 1,5diphenyl-3,7-bis(methoxyalkyl)bispidin-9-ones (I) were prepd. by a general reaction from 1,3-diaryl-2-propanone, paraformaldehyde, and primary amine acetates.

A mixt. of 0.1 mole 1,3diphenyl-2-propanone, 0.4 mole paraformaldehyde, 0.1 mole RNH₂.AcOH, and 0.1 mole R'NH₂.AcOH in 100 ml. alc. was refluxed 6-42 hrs., according to the employed amine, cooled, dild. with equal vol. H₂O, alkalized to pH 8-9 with 20% Na₂CO₃, kept overnight in the cold, filtered, and the ppt. crystd., if solid or purified through perchlorates and hydrochlorides, if liquid. The following sym. I were prepd. (salt, R = R', m.p., and % yield given): -, (CH₂)₂OCH₃, 90-1.degree., 71; -, (CH₂)₃OCH₃, 78-9.degree., 53; perchlorate 0.5-H₂O, (CH₂)₃OH, 94-6.degree. (anhyd. m. 148-9.degree.), 47; -, (CH₃)₂CCH₂OH, 187-8.degree., 34; hydrochloride, (CH₂)₃OH, 191-3.degree. (decompn.), 36; perchlorate, 3,4,5-trimethoxyphenethyl, 204-6.degree., 35. The asym. I were obtained (R, R', m.p., and % yield given): (CH₂)₂OCH₃, CH₂Ph, 101-3%, 42; (CH₂)₃OCH₃, cyclopentanyl, 118-20.degree., 35. The ir spectra were reported. Also reported were the results of preliminary toxicological tests, which showed that the activity of I decreased rapidly with increasing of length of the substituent chain in the 3- and 7-position.

IT **4208-17-7**, 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclohexyl-7-ethyl-1,5-diphenyl- **4208-32-6**, 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dicyclohexyl-1,5-diphenyl- **4478-45-9**, 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclopentyl-7-(3-methoxypropyl)-1,5-diphenyl- (prepn. of)
 RN 4208-17-7 CAPLUS
 CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclohexyl-7-ethyl-1,5-diphenyl- (7CI, 8CI) (CA INDEX NAME)

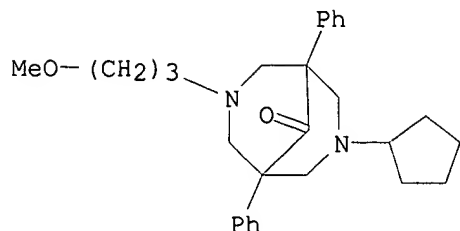


RN 4208-32-6 CAPLUS
 CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dicyclohexyl-1,5-diphenyl- (6CI, 7CI, 8CI) (CA INDEX NAME)



RN 4478-45-9 CAPLUS
 CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3-cyclopentyl-7-(3-methoxypropyl)-1,5-

diphenyl- (7CI, 8CI) (CA INDEX NAME)



ANSWER 28 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1965:90941 CAPLUS

DOCUMENT NUMBER: 62:90941

ORIGINAL REFERENCE NO.: 62:16251g-h,16252a

TITLE: Synthesis of 1,5-diphenylbispidin-9-ones. VII.
Symmetrical 1,5-diphenyl-3,7-dialkylbispidonesAUTHOR(S): Chiavarelli, Stefano; Toeffler, Federico; Vittory,
Rodolfo Landi; Mazzeo, Pietro

CORPORATE SOURCE: Ist. Super Sanita, Rome

SOURCE: Gazz. Chim. Ital. (1964), 94(10), 1021-7

DOCUMENT TYPE: Journal

LANGUAGE: Italian

GI For diagram(s), see printed CA Issue.

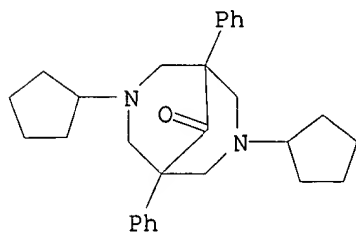
AB cf. CA 56, 12900c. Correction of CA 62, 9135h. The title compds. (I) were obtained by the Mannich reaction on (PhCH₂)₂CO (II) and a primary or cycloalkylamine acetate in the presence of CH₂O. Thus, 12.6 g. II, 7.2 g. CH₂O, and 21 g. heptylamine acetate in 100 ml. MeOH refluxed 17 hrs. gave 45% I (R = C₇H₁₅) perchlorate, m. 122-4.degree. (MeOH). Similarly were obtained the following I (R, % yield, and m.p. given): C₈H₁₇, 51, --(HClO₄ salt m. 116-18.degree.); iso-C₈H₁₇, 58, 89-91.degree.; C₁₀H₂₁, 38, --(HClO₄ salt m. 126-8.degree.); C₁₇H₃₅, 69, 67-8.degree.; C₁₈H₃₇,

56, 56-8.degree.; cyclopentyl, 62, 156-8.degree..

IT **3168-98-7**, 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dicyclopentyl-1,5-diphenyl- (prepn. of)

RN 3168-98-7 CAPLUS

CN 3,7-Diazabicyclo[3.3.1]nonan-9-one, 3,7-dicyclopentyl-1,5-diphenyl- (7CI, 8CI) (CA INDEX NAME)



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L3 6 S L1
L4 STRUCTURE UPLOADED
L5 QUE L4
L6 5 S L4
L7 100 S L6 FUL

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L8 28 S L7

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ENTRY

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